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Contribution to the development of a dynamic Life Cycle Assessment method

Allan Shimako

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THÈSE

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English abstract

Life Cycle Assessment (LCA) is the most widely used method for the environmental evaluation of an anthropogenic system and its capabilities no longer need to be proved. However, several limitations have been pointed out by LCA scholars, including the lack of a temporal dimension. The processes of technosphere are dynamic and successive in time which leads to a time dependent life cycle inventory (LCI). Environmental mechanisms involved in impact developments have distinct dynamic behaviours determining specific temporal occurrence. However, the current life cycle impact assessment (LCIA) methods consider arbitrarily fixed time horizons and/or steady state conditions.

The objective of this thesis is to contribute to the development of an operational methodology and adapted tools for the consideration of time dependency in LCA, with strong emphasis on the development of an integrated modelling solution for both the life cycle inventory and the life cycle impact assessment phases. This work is part of the ANR-FNR project DyPLCA. In this project and previously to the thesis work, a mathematical model and software were developed for temporal LCI calculation. They were used for parallel developments of a temporal database and dynamic LCIA methods.

The first contribution of this thesis concerns the development of a temporal data base, leaning againstecoinvent data base, in which temporal parameters (defined in the DyPLCA temporal LCI model) have been attributed to the data sets in the activity sectors of chemical/biochemical processes and waste treatment.

Dynamic climate change and toxicity impacts were developed by adapting available models and were implemented in a homemade computational tool. The modelling approach takes into account the noisy nature of substance emissions in function of time like in the real world) as calculated by DyPLCA temporal LCI model.

In the case of dynamic climate change, IPCC available models (impulse response functions) and data for different greenhouse gases (GHG) were used in order to calculate time dependent radiative forcing and mean temperature change, independently of a time horizon. Concerning dynamic toxicity, this work focuses on the dynamic fate model for substances in the environment (Simplebox model solved by adapted numerical methods) which was combined with the USEtox[®] model for human toxicity/ecotoxicity assessment. The results are expressed as time dependent toxicity values (USEtox units/time).

The modelling framework, i.e. dynamic LCI coupled with dynamic LCIA, was applied to relevant case studies in order to emphasize the features of the new approach. In addition, the results were compared to conventional LCA results.

Keywords: dynamic LCA, life cycle inventory, climate change, toxicity, ecotoxicity

Résumé en Français

L'analyse du cycle de vie (ACV) est la méthode la plus utilisée pour l'évaluation environnementale d'un système anthropique et ses capacités n'ont plus besoin d'être prouvées. Cependant, les spécialistes ont souligné plusieurs limites de cette méthode, dont l'absence de dimension temporelle. Les procédés de la technosphère sont dynamiques et ils se succèdent dans le temps, ce qui conduirait à un inventaire de cycle de vie (ICV) dépendant du temps. Les mécanismes environnementaux impliqués dans la génération des impacts ont des caractéristiques dynamiques variées déterminant une manifestation temporelle spécifiques des impacts. Cependant, les méthodes d'évaluation des impacts du cycle de vie (EICV) actuelles considèrent des conditions stationnaires et des horizons de temps arbitrairement fixés.

L'objectif de cette thèse est de contribuer au développement d'une méthodologie opérationnelle et des outils adaptés pour la prise en compte de la dépendance temporelle dans l'ACV, en accordant une importance particulière au développement d'une approche de modélisation intégrée pour les phases de l'ICV et l'EICV. Ce travail fait partie du projet ANR-FNR DyPLCA. Dans ce projet et précédemment au travail de thèse, un modèle mathématique et un logiciel ont été développés pour le calcul de l'ICV temporel, qui ont été utilisés pour le développement parallèle d'une base de données temporelle et des méthodes d'EICV dynamiques.

La première contribution de cette thèse concerne le développement d'une base de données temporelle, en s'appuyant sur la base de donnéesecoinvent, dans laquelle les paramètres temporels (définis dans le modèle d'ICV temporel DyPLCA) ont été attribués aux sets de données des secteurs d'activité des procédés chimiques / biochimiques et des traitements des déchets.

Des indicateurs dynamiques pour les impacts changement climatique et toxicité ont été développés en adaptant les modèles disponibles et ils ont été mis en place dans un outil de calcul propre. L'approche de modélisation tient compte de la nature fluctuante des émissions des substances en fonction du temps (comme dans le monde réel), calculées par le modèle d'ICV temporel DyPLCA.

Dans le cas du changement climatique dynamique, les modèles disponibles de l'IPCC (les fonctions de réponse impulsionnelle) et les données pour différents gaz à effet de serre (GES) ont été utilisés pour calculer le forçage radiatif dynamique et le changement de température moyen, sans faire appel à un horizon de temps. En ce qui concerne la toxicité dynamique, ce travail se concentre sur le modèle dynamique du devenir des substances dans l'environnement (modèle Simplebox résolu par des méthodes numériques adaptées) qui a été combiné avec le modèle USEtox[®] pour l'évaluation de la toxicité humaine et de l'écotoxicité. Les résultats sont exprimés en valeurs de toxicité en fonction du temps (unités USEtox / temps).

L'approche de modélisation, i.e. l'ICV dynamique associé à l'EICV dynamique, a été appliquée à des cas d'études pertinents afin de mettre en évidence les caractéristiques de la nouvelle approche. De plus, les résultats ont été comparés aux résultats conventionnels de l'ACV.

Mots-clés: ACV dynamique, inventaire du cycle de vie, changement climatique, toxicité, ecotoxicité
Scientific production

Résumé étendu

L'analyse du cycle de vie (ACV) est la méthode la plus utilisée pour l'évaluation environnementale des systèmes anthropiques et ses capacités n'ont plus besoin d'être prouvées. Cependant, les spécialistes dans ce domaine ont souligné plusieurs limites de cette méthode, dont l'absence de dimension temporelle. Les procédés de la technosphère sont dynamiques et ils se succèdent dans le temps, ce qui conduirait à un inventaire de cycle de vie (ICV) dépendant du temps. Les mécanismes environnementaux impliqués dans la génération des impacts ont des caractéristiques dynamiques variables ce qui détermine une manifestation temporelle spécifiques des impacts. Cependant, les méthodes d'évaluation des impacts du cycle de vie (EICV) actuelles considèrent des conditions stationnaires et des horizons de temps arbitrairement fixés.

Les caractéristiques temporelles sont essentielles pour décrire le fonctionnement des procédés complexes (par exemple, les procédés biotechnologiques, les bâtiments, les transports, etc.) et leurs impacts. L'émission de substances nuisibles à l'environnement par les activités d'un système de production est fondamentalement dynamique. Les caractéristiques dynamiques de ces émissions dépendent de la nature des activités, de la chaîne d'approvisionnement, des stocks, de la saisonnalité, des décalages temporels, etc. Les impacts causés par les émissions sont également dynamiques. Le changement climatique, la dégradation de la couche d'ozone, l'acidification, la toxicité humaine et l'écotoxicité sont quelques exemples. Ils ont également un comportement temporel spécifique qui dépend des différentes conditions environnementales telles que le transfert de masse, les réactions chimiques ou biologiques, etc.

Les études menées pour la considération de la dimension temporelle dans l'ACV n'incluent généralement que la dynamique dans une seule étape de l'ACV ou ils sont simplifiés en ne tenant pas compte de toutes les substances présentes dans le cas d'étude.

L'objectif de cette thèse est de contribuer au développement d'une méthodologie opérationnelle et des outils adaptés pour la prise en compte de la dépendance temporelle dans l'ACV, en accordant une importance particulière au développement d'une approche de modélisation intégrée pour les phases d'ICV et EICV.

Le travail de recherche présenté dans cette thèse de doctorat fait partie d'un projet de recherche appelé DyPLCA (Dynamic Processes Life Cycle Assessment) financé par l'agence de recherche nationale française (ANR) et l'agence de recherche nationale luxembourgeoise (FNR). La thèse a été réalisée au Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP), Toulouse. Dans ce projet et précédemment au travail de thèse, un modèle mathématique et un logiciel ont été développés pour le calcul de l'ICV temporel, qui ont été utilisés pour le développement parallèle d'une base de données temporelle et des méthodes d'EICV dynamiques. L'approche développée est compatible avec les

outils et les méthodes actuels d'ACV conventionnel afin de permettre son utilisation par les praticiens de l'ACV.

L'adaptation d'une base de données d'ACV a été faite pour prendre en compte des paramètres temporels dans le calcul de l'ICV. Dans cette thèse, des paramètres temporels ont été attribués aux procédés chimiques, biochimiques et de traitement des déchets. Cette base de données temporelles, associée à ecoinvent v3.2, est nécessaire pour construire le réseau de procédés du cycle de vie et pour résoudre le modèle d'ICV dynamique pour les procédés d'arrière-plan. Les procédés ayant des caractéristiques particulières par rapport au modèle générique d'ICV dynamique ont été identifiés et des modifications au modèle génériques ont été proposées. Plusieurs propositions ont déjà été implémentées dans l'outil web DyPLCA.

En ce qui concerne l'indicateur de réchauffement climatique dynamique, deux indicateurs d'impact dynamique ont été développés : le changement de température moyenne et le forçage radiatif. Premièrement, les méthodes conventionnelles ont été présentées et ensuite la base pour le développement des métriques dynamiques a été expliquée. Les résultats d'impact sont obtenus en tant que valeurs d'indicateur pour n'importe quel moment. La méthode proposée est flexible ne nécessitant pas d'horizon temporel fixé, contrairement à l'ACV classique. La méthode n'utilise pas de facteurs de caractérisation (établis pour une émission impulsionnelle unitaire au temps zéro et pour un horizon temporel fixé), mais elle calcule les indicateurs d'impact en fonction de la charge atmosphérique réelle déterminée par un profil temporel d'émission donné selon le cas d'étude. Les modèles dynamiques ont été appliqués dans un cas d'étude (production de bioénergie à partir de microalgue), ce qui a permis d'analyser et discuter les aspects temporels du réchauffement climatique et de l'ICV dynamique.

Pour calculer les impacts de toxicité dynamique, le modèle USEtox® a été choisi et adapté pour inclure la dimension temporelle. Parmi les étapes de calcul de la toxicité, les aspects temporelles ont été étudiés dans le calcul du devenir des substances dans les différents compartiments de l'environnement. Les résultats ont montré que la nature des substances a une importante influence dans les résultats de la toxicité. Les substances organiques tendent à être relativement rapidement éliminées des compartiments environnementaux et leur devenir suit une évolution similaire dans le temps au flux d'émission. Les substances inorganiques sont pour la plupart persistantes et accumulées dans certains compartiments, leur potentiel de toxicité dure pendant des siècles. Ces caractéristiques ne sont pas mises en évidence dans l'ACV conventionnelle. La méthode développée a été appliquée à un cas d'étude, à savoir la production de raisins, afin de mettre en évidence les résultats de l'approche proposée. Ce cas d'étude a été choisi pour diverses raisons: i) l'agriculture utilise des substances potentiellement dangereuses dans les différentes étapes de la production, de sorte qu'une analyse temporelle de l'ICV et des impacts environnementaux est justifiée; ii) diverses substances sont émises dans l'environnement par des opérations agricoles, c.-à-d. des métaux et des composés organiques ayant différents types d'effets nocifs sur les êtres humains et les écosystèmes.

Une analyse de sensibilité des différents paramètres temporels sur le résultat de calcul d'impact a été réalisée. L'une des questions principales est de savoir comment le détail de la définition temporelle de l'inventaire influencera les résultats finaux de l'ACV. Dans ce but, l'analyse de sensibilité a été réalisée sur un cas d'étude : le cycle de vie du traitement des eaux usées. Le choix du cas d'étude a été guidé par la variabilité temporelle élevée des paramètres physiques impliqués dans ce procédé, conduisant à un profil temporel complexe de l'ICV.

Enfin, l'approche complète composée de la dernière version de l'application web DyPLCA connectée à la base de données temporelle, la base de données ecoinvent et le calcul dynamique des impacts, a été appliquée pour un cas d'étude (différents scénarios du mix d'électricité de 2010 à 2070 en France). Cette application a démontré le fonctionnement de l'ensemble des outils développés et la faisabilité de l'ACV dynamique.

Ce travail de thèse a fourni des outils pour les deux étapes d'ACV (l'ICV et l'EICV) et leur couplage pour une ACV dynamique complète. De plus, les outils et méthodes développés permettent leur utilisation par les praticiens de l'ACV classique sans devoir gérer de changements drastiques par rapport à la méthode conventionnelle.

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Scientific papers published in international and peer reviewed journals

- Shimako, A. H., Tiruta-Barna, L., Pigné, Y., Benetto, E., Gutiérrez, T. N., Guiraud, P. & Ahmadi, A. (2016). Environmental assessment of bioenergy production from microalgae based systems. *Journal of Cleaner Production*, 139, 51-60.
- Shimako, A.H., Tiruta-Barna, L. & Ahmadi, A. (2017). Operational integration of time dependent toxicity impact category in dynamic LCA. *Science of The Total Environment*, 599, 806-819.
- Shimako, A.H., Tiruta-Barna, L., Bisinella de Faria, A.B., Ahmadi, A., Spérandio, M. (2017). Sensitivity analysis of temporal parameters in a dynamic LCA framework (in preparation)

Conferences with abstract

- Shimako, A. H., Tiruta-Barna, L., Pigné, Y., Benetto, E., Gutiérrez, T. N., Guiraud, P., & Ahmadi, A. 2015. Environmental assessment of energy production from microalgae based systems ECCE 10 + ECAB 3 + EPIC 5 (oral).
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- Shimako, A. H., Bisinella De Faria, A.B., Tiruta-Barna L., Ahmadi, A., Sperandio, M., 2016. Dynamic Life Cycle Assessment applied to a wastewater treatment plant construction and operation. SETAC Europe LCA CSS Montpellier (poster).

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List of abbreviations

ADEME	French Environment and Energy Management Agency
AGTP	Absolute Global Temperature Potential
AGWP	Absolute Global Warming Potential
ANR	French national research agency
AOGCM	Atmosphere-Ocean General Circulation Models
BAF	Bioaccumulation Factor
CED	Cumulative Energy Demand
CF	Characterization Factor
CSTB	Centre Scientifique et Technique du Bâtiment
DLCA	Dynamic Life Cycle Assessment
EB	Energy Balance
EC50	Concentration for which 50% of the population is affected
EF	Effect Factor
EQ	Ecosystem Quality
EROI	Energy Return On Investment
FF	Fate Factor
FNR	Luxembourg national research agency
FU	Functional Unit
GHG	Greenhouse Gases
GHG	Greenhouse Gas
GTP	Global Temperature Potential
GWP	Global Warming Potential
HC50	Hazardous concentration at which half of the target population is exposed
HH	Human Health
IEA	International Energy Agency
IOA	Input/output analysis
IPCC	Intergovernmental Panel on Climate Change
IR	Ingestion Rate
IRF	Impulse Response Function
ISIC	International Standard Industrial Classification of All Economic Activities
ISO	International Organization for Standardization
IUCN	International Union for Conservation of Nature
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory

LCIA	Life Cycle Impact Assessment
LISBP	Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés
LIST	Luxembourg Institute of Science and Technology
LITIS	Laboratoire d'Informatique, du Traitement de l'Information et des Systèmes
MEST	Ministry of Ecological and Solidarity Transition
MFA	Material flux analysis
MM	Molar Weight
ODE	Ordinary Differential Equations
PAF	Potentially Affected Fraction
R	Resources
RED	Renewable Energy Directive
RF	Radiative Forcing
SAR	IPCC Second assessment Report
SETAC	Society for Environmental Toxicology and Chemistry
SI	Supplementary Information
TH	Time Horizon
UNCED	United Nations Conference on Environment and Development
UNEP	United Nations Environment Program
UNFCCC	United Nations Framework Convention on Climate Change
WWTP	Wastewater Treatment Plant
XF	Exposure Factor

**Chapter I. General
introduction: Life cycle
assessment and sustainable
development**

Résumé

Le concept de développement durable a été abordé pour la première fois en 1969 dans le nouveau mandat adopté par l'Union Internationale pour la Conservation de la Nature (UICN, Adams, 2006). Ensuite, le développement durable a été un sujet de discussion clé dans la Conférence des Nations Unies sur l'Environnement Humain à Stockholm en 1972 (UN, 1972). L'une des principales définitions du développement durable a été évoquée en 1987 dans le rapport « Our Common Future » (Brundtland, 1987) qui est connu sous le nom de Rapport Brundtland. Le développement durable est défini comme le «développement qui répond aux besoins du présent sans compromettre la capacité des générations futures à répondre à leurs propres besoins».

En ce qui concerne les préoccupations environnementales, les premiers signes majeurs datent de 1962 lorsque Rachel Carson, dans le livre «Silent Spring », souligne les effets négatifs des pesticides sur l'environnement. Sa publication met en garde le public sur le danger de l'utilisation des pesticides dans l'agriculture. De plus, elle soutient que notre capacité à changer l'environnement doit être utilisée avec une prudence maximale pour ne pas mettre en danger le système auquel nous appartenons.

La réglementation et le contrôle des activités humaines qui ont potentiellement des effets néfastes sur l'environnement sont devenus une nécessité. Pour cette raison, plusieurs outils et méthodes ont été développés afin d'évaluer l'influence des systèmes de production sur l'environnement. Parmi ces méthodes, l'Analyse du Cycle de Vie (ACV) est l'une des plus acceptées et utilisées pour l'évaluation environnementale des activités anthropiques.

L'ACV est une méthode qui calcule les impacts potentiels associés aux produits, aux procédés et aux services sur leur cycle de vie entier (c.-à-d. du berceau à la tombe). Les normes ISO 14040-14044 précisent les consignes pour la réalisation d'une étude d'ACV (ISO, 2006a, ISO, 2006b). L'utilisation de cette méthode est encouragée, l'Union Européenne, l'Australie, le Canada, la Corée, le Japon et les États-Unis utilisent l'ACV comme un élément principal pour la politique environnementale (Guinee et al., 2010).

L'ISO 14040-14044 (2016a; 2016b) établit l'étude d'ACV en quatre étapes: la définition de l'objectif et des frontières, la construction de l'Inventaire du Cycle de Vie (ICV) en fonction des bilans de masse et d'énergie sur l'ensemble du cycle de vie du système, l'Évaluation de l'Impact du Cycle de Vie (EICV) en fonction de différents modèles de calcul d'impact et l'étape d'interprétation (ISO, 2006a, ISO, 2006b).

Dans l'étape de définition de l'objectif d'ACV, les informations générales du projet sont décrites. La problématique, les objectifs et la portée de l'étude sont définis. L'objectif d'une étude d'ACV est de

définir le point de vue, le public cible et sa pertinence. La portée d'une étude d'ACV tient compte de ses aspects temporels et géographiques et de sa couverture technologique.

En ce qui concerne l'ICV, deux techniques existent pour la résolution de calcul d'inventaire d'ACV (Heijungs et Suh, 2002). L'approche séquentiel commence par les procédés de l'unité fonctionnelle et se déroule linéairement à travers la chaîne d'approvisionnement pour les procédés et les produits requis. L'approche matricielle considère l'ACV comme un système d'équation linéaire qui peut être résolu par l'algèbre linéaire (Heijungs 1994, Heijungs et Suh 2002).

L'étape d'EICV convertit l'émission des substances et l'extraction des ressources naturelles en impacts environnementaux. Dans cette étape, des méthodes et des modèles sont utilisés pour calculer des facteurs de caractérisations (Pennington et al., 2004). Les méthodes utilisées dans l'EICV peuvent être divisées en deux catégories: orientées problème et orientées dommage.

L'étape d'interprétation d'une étude d'ACV consiste principalement en la vérification de la cohérence et complétude; analyse de contribution et de gravité; analyse d'incertitudes et de sensibilité; conclusions et recommandations (Guinée et al., 2002).

Plusieurs améliorations ont été apportées à la méthode d'ACV afin d'assurer la qualité des résultats à venir. Malgré tous les efforts pour son développement, la méthode ACV présente encore des limitations. Finnveden (2000), Reap et al. (2008) ont soulevé des problèmes tels que la qualité des données, l'allocation, l'incertitude, la prise en compte du temps et de la localisation, etc.

L'objectif principal de cette thèse est de contribuer au développement d'une approche complète d'ACV dynamique, par le développement d'une méthode, des modèles et des outils de calcul. La méthode prendrait en compte les caractéristiques temporelles dans les étapes de l'inventaire (ICV) et de l'évaluation d'impact (EICV). L'approche développée doit être compatible avec les outils et les méthodes actuels d'ACV conventionnel afin de permettre son utilisation par les praticiens de l'ACV.

Le travail de recherche présenté dans cette thèse fait partie du projet de recherche DyPLCA (Dynamic Processes Life Cycle Assessment) financé par l'agence de recherche nationale française (ANR) et l'agence de recherche nationale luxembourgeoise (FNR). Le travail a été réalisé au Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP), Toulouse.

I.1. Sustainable development: finding the balance towards the Earth

“Sustainable development is the pathway to the future we want for all. It offers a framework to generate economic growth, achieve social justice, exercise environmental stewardship and strengthen governance.”

Ban Ki-moon

Technology at present is an inherent part of the human culture. Its development is ever more rapid since the industrial revolution. Equipment, machines, products have been used to facilitate human tasks which increases the efficiency of production as well as the well-being of society. However, all those advantages came in exchange of environmental wellness. After the technological boost provided by industrial revolution in 1700s, the impacts caused by human activity in environment were neglected by governments and industries. Mass production systems and the technologies used by humans were and still are responsible of a big share in many environmental impacts such as toxicity, ozone depletion, climate change.

It was only in 1969 that the concept of sustainable development was widely discussed in the new mandate adopted by the International Union for Conservation of Nature (IUCN; Adams, 2006). Then, sustainability was a key point of discussion in the United Nations Conference on the Human Environment in Stockholm 1972 (United nations, 1972).

One of the main definitions of sustainability was evoked in 1987 in the Our Common Future Report (Brundtland, 1987) most known as Brundtland Report. It claims that sustainable is the “development that meets the needs of the present without compromising the ability of future generations to meet their own needs”.

“In essence, sustainable development is a process of change in which the exploitation of resources, the direction of investments, the orientation of technological development and institutional change are all in harmony and enhance both current and future potential to meet human needs and aspirations.” Brundtland, 1987

However, Workshop on Urban Sustainability of the US National Science Foundation (2000) pointed out that nowadays the concept of sustainability is ‘laden with so many definitions that it risks plunging into meaninglessness, at best, and becoming a catchphrase for demagoguery, at worst’.

However, neglecting the fact that the human activity has harmful impacts on the environment is a mistake. The degradation of environment is already affecting millions of people in developing countries and is likely to degrade the human well-being across the globe within the next centuries (Lélé, 1991).

The IUCN Programme (Adams, 2006) demonstrates the three objectives of sustainable development as interlocking circles representing the economy, the society and the environment. The theoretical idea of sustainability is the one in which the economic, social and environmental needs have to be addressed with the same importance (Figure II.1.A). However, in the current situation of the world, economical efforts overpower the social and environmental ones (Figure II.1.B) due to the fast economic growth and importance and also the disregard of the environment in the past.

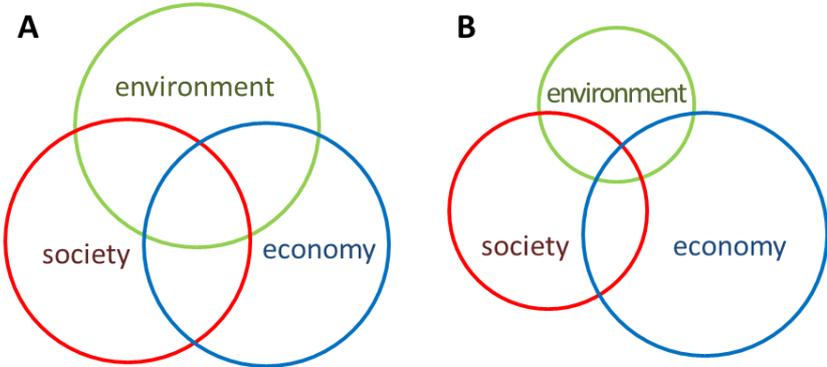


Figure II.1 – Sustainable development objectives. A – theoretical and B – current situation of objectives.

However, this model is usually subject of debate among analysts. The representation of a green economics is different: the economy, at first, is part of human society which, finally, is part of the environmental system (Figure II.2; Cato, 2009).

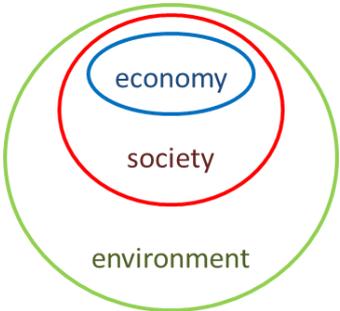


Figure II.2 – Green economic vision of the system composed by economy, society and environment.

As economy and society belongs to environment, taking care of the latter is essential for the development of all. The economical and societal interests have to respect the limits imposed by the

environment. Humanity future may be in danger if the trade between human activities and environmental capacity are unbalanced. Therefore, Brundtland (1987) states that “our inability to promote the common interest in sustainable development is often a product of the relative neglect of economic and social justice within and amongst nations”.

1.1.1. Environmental sustainability

“The environment is everything that isn’t me.”

Albert Einstein

Environmental awareness has been growing as the harmful effect of human actions is becoming more evident in the environment. Climate change, ozone depletion, water contamination are few examples of impacts in environment which the human activity play a part in. Even though some claim that those would naturally happen, human activity is accelerating the impact which may not allow the adaptation of environment to the future conditions.

“Humanity must learn to live within the limitations of the biophysical environment. Environmental sustainability means natural capital must be maintained, both as a provider of inputs (‘sources’), and as a ‘sink’ for wastes.” Goodland, 1995

Human awareness towards the environment is recent. The first major reported evidence of environment concerns dates from 1962 when Rachel Carson in the book *Spring* highlights the harmful effects of pesticides on the environment. Her publication warns general public showing the opinion of experts on the danger of pesticides use in agriculture. Also, she argues that our ability to change the environment has to be used with maximum prudence not to endanger the system that we belong. More than 2 decades after, a big step towards environmental sustainability was made by the United Nations in 1987 in their report “Our Common Future”.

Many other agreements looking forwards the protection of environment were held during the last decades. United Nations Conference on Environment and Development (UNCED), most known as “Rio Earth Summit”, was a major environmental conference which envisaged making progress envisaging sustainable development. This conference aims were based in the outcomes of the Brundtland Report which envisaged to look after the most important environmental problems and settle major treaties on biodiversity, climate change and forest management. The conference was held in 1992 and was divided in different conventions such as Convention on Biological Diversity, Convention on Climate Change, and Convention on the Law of the Sea, some related to toxicity which different themes of discussion.

For example, United Nations Framework Convention on Climate Change (UNFCCC) has as objective to stabilize the greenhouse gases concentration to a level in which anthropogenic interference is not dangerous to the climate system (ecosystems adaptation, food production, etc.). The well-known Kyoto Protocol (1997) was a treaty among 192 countries which extend the UNFCCC.

Regulating and controlling human activities that potentially have harmful impacts in environment become a necessity. For this reason, several tools and methods were developed in order to evaluate the influence of production systems on environment, among which we can cite:

- Material flux analysis - MFA (Brunner and Rechberger, 2004)
- Input/output analysis – IOA (Suh, 2009)
- Carbon footprint (Wiedmann and Minx, 2008)
- Environmental risk assessment (Burgess and Brennan, 2001)
- Environmental impact assessment (Burgess and Brennan, 2001)
- Cost benefit analysis (Pearce, 1998)

Life Cycle Assessment - LCA (ISO, 2006a; ISO, 2006b) with its variants: Environmental assessment, Social assessment, life cycle Cost assessment.

Among these methods, Life Cycle Assessment (LCA) is one of the most accepted and used for the environmental assessment of anthropogenic activities.

I.2. Life cycle assessment for sustainability assessment

Life Cycle Assessment (LCA) is a method that calculates potential impacts associated with products, processes and services over their entire life cycle (i.e. cradle-to-grave).

ISO standards 14040-14044 specify the guide for conducting a LCA study (ISO, 2006a; ISO, 2006b). The use of this method is encouraged by many governments. European Union, Australia, Canada, Korea, Japan and the USA use LCA as main element in environmental policy (Guinee et al., 2010).

“The purpose of LCA is to compile and evaluate the environmental consequences of different options for fulfilling a certain function.” (Guinée et al., 2002)

The first LCA study is attributed to Harry E Teastley Jr in 1969 in which, in his work to Coca-Cola, he performed an environmental assessment for the comparison between a plastic and glass bottle, from

the raw material to the end-of-life (recycling or incineration). Only the summary of this study was published in “Science Magazine” and no complete report was released (Hunt and Franklin, 1996).

LCA has only been widely used since the beginning of 1990s. At this period, Heijungs et al. (1992) published a first “schema” in which the possible steps of an environmental analysis are described. Then, the Society of Environmental Toxicology and Chemistry (SETAC) released the guide “Guidelines for Life-cycle Assessment: A code of practice” in 1993 which aimed to present the general principles and framework for a LCA study. Finally, the International Organization for Standardization (ISO) constituted an international standard for LCA. The principles and framework for a LCA study are described in ISO 14040 and the requirements and guidelines are presented in ISO 14044 (ISO 2006a, 2006b).

ISO 14040-14044 (2016a; 2016b) divides a LCA study in four steps (Figure II.3): the definition of the goal and scope, the construction of the Life Cycle Inventory (LCI) based on mass and energy balances over the whole system life cycle, the Life Cycle Impact Assessment (LCIA) based on various impact calculation models, and the interpretation step (ISO, 2006a; ISO, 2006b).

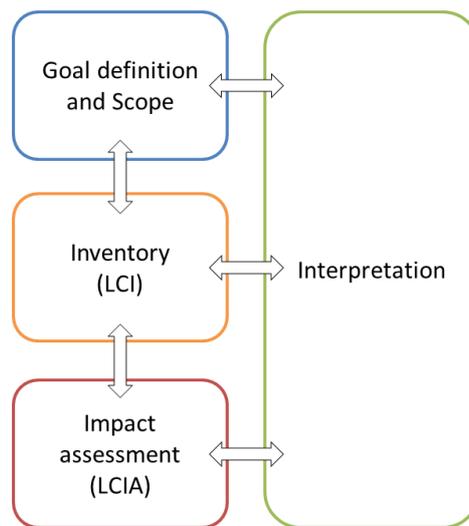


Figure II.3 – LCA steps: Goal and scope definition, inventory, impact assessment and interpretation.

1.2.1. Goal and scope definition

In the goal and scope definition step of LCA, the general information of the project is described. The problematic, objectives and scope of the study are defined. It is in this step where the functional unit (FU) and reference flows of the LCA study are defined. The FU describes the quantity of the production system being investigated. Functional unit is the specification in LCA that allows the products or services to be compared and analysed (Rebitzer et al. 2004). In theory, modelling a LCA study should comprise all processes in the life cycle of a service or product. However, it is impractical

to consider all the processes involved in one production system. For this reason, the boundaries and limits of the studied system have also to be defined.

1.2.2. Life Cycle Inventory

The Life Cycle Inventory (LCI) step consists in the quantitative description of the production system. In this step the system boundaries, the flow diagrams, the data collection and allocation are established. The inputs from and outputs to environment which are correlated to a functional unit are accounted (Guinée et al., 2002). This is the most laborious step: all the flows in the studied system are cautiously accounted, i.e. hundreds to thousands of services, products, environmental interventions.

Currently, sequential method and matrix are the two broad techniques for the computational resolution of LCA inventory (Heijungs and Suh 2002). The calculation in the sequential approach starts with the functional unit processes and goes linearly through the supply chain for the required processes and products. The matrix approach considers the LCA as a system of linear equations which can be solved by linear algebra (Heijungs 1994, Heijungs and Suh 2002).

Considering the matrix resolution of LCI, the studied system can be represented by a system of linear equations (Equation II.1):

$$\mathbf{s} = \mathbf{A}\mathbf{s} + \mathbf{f} \quad \text{Equation II.1}$$

The technological matrix \mathbf{A} represents the exchange between processes. It corresponds to a matrix with zeros on its diagonal. The values $a_{i,j}$ in the matrix represent the quantity of process i (represented in the row) necessary for the production of a unit of output of process j (represented in the column) (Suh and Huppes, 2005). Finally, the vector \mathbf{s} can be calculated by:

$$\mathbf{s} = (\mathbf{I} - \mathbf{A})^{-1}\mathbf{f} \quad \text{Equation II.2}$$

where \mathbf{I} denotes the identity matrix.

The inventory results (\mathbf{g}) are then calculated by the multiplication of \mathbf{s} by the matrix of environmental interventions \mathbf{B} (Equation II.3):

$$\mathbf{g} = \mathbf{B}\mathbf{s} \quad \text{Equation II.3}$$

Matrix \mathbf{B} contains the elements $b_{k,i}$ which are direct emissions or natural resources withdrawn by the process i . The resultant vector \mathbf{g} represents the elementary flows linked to the production system being studied, i.e. the LCI of the system.

LCA databases were developed in order to simplify the collection of adequate and reliable data for thousands of processes. Ecoinvent, Gabi, ESU World food are examples of general databases available for use in LCA, with additional national data bases developed in several countries (Japan, USA, Canada, Germany, Italy, Switzerland, and Sweden; Rebitzer et al., (2004)).

Ecoinvent v.3 is the current version of ecoinvent (Wernet et al., 2016). It contains thousands of activities in different economic sectors such as manufacturing, construction, agriculture, forestry and fishing, mining and quarrying, etc. They can be divided in different economical sector following the International Standard Industrial Classification of All Economic Activities (ISIC; United Nations, 2008). Data in ecoinvent are available in two different forms: system (flux of emissions and resources) and Unit (detailed data per processes). Also, multiple processes are handled in three different form in ecoinvent: allocation, cut-off by classification (by-products are classified as recyclable), allocation at the point of substitution (by-products considered to be part of the waste producing system) and substitution, consequential, long-term (by-products handled by system expansion). Moreover, the quality of data is provided by the pedigree matrix (Weidema and Wesnaes, 1996).

1.2.3. Life Cycle Impact Assessment

The Life Cycle Impact Assessment (LCIA) step converts the elementary flows into impacts on environment. This step is based on methods and models for the calculation of specific indicators associated to the substances and impact categories (Pennington et al., 2004).

The indicators at midpoint level (such as acidification, climate change and ecotoxicity) represent a problem oriented approach while the indicators at endpoint level represent damages on areas of protection (human health, ecosystem quality, resource depletion).

One of the key principles of the LCA method is the use of characterization factors CF, i.e. constants specific for a given substance/impact/environmental compartment. CFs are then used for impact calculation by the simple linear relation between the substance inventory g_s and its CF:

$$\text{Impact result} = \mathbf{g}_s \mathbf{CF}_s \quad \text{Equation II.4}$$

Different methods were developed for the calculation of characterization factors for various impact categories, for midpoint and endpoint evaluations, for example CML, Ecoindicator99, Impact2002+, ReCiPe, etc. These methods are available with LCA databases and software.

Pennington et al. (2004) illustrated the potential variables of non-generic characterization factor in the case of impacts on human health and the natural environment:

$$CF(s, i, t) = \sum_j \frac{Effect(s, j, t)}{Emission(s, i)}$$

$$= \sum_j \left(\frac{Fate(s, j, t)}{Emission(s, i)} \right) \cdot \left(\frac{Exposure(s, j, t)}{Fate(s, j, t)} \right) \cdot \left(\frac{Effect(s, j, t)}{Exposure(s, j, t)} \right) \quad \text{Equation II.5}$$

In this general formulation, *s* represents the substance, *i* the location of emission, *j* the location of exposure and *t* is the time period during which the potential contribution to the impact is taken into account. However, in LCA those variables are often only partially considered or ignored (Pennington et al., 2004).

This general model was transposed in LCIA methods for toxicity and ecotoxicity impacts. Midpoint characterization factors (CF_m) are calculated by the multiplication of fate, exposure and effect factors. When considering many environmental compartments, a matrix approach is useful:

$$CF_{m,s} = EF_s \times XF_s \times FF_s \quad \text{Equation II.6}$$

where *FF* is the matrix of fate factors, *XF* is the matrix of exposure factor and *EF* is the matrix of effect factor. CF_m is a vector in which every element cf_i represents the midpoint characterization factor for the substance *s* in the compartment *i*.

In all LCIA methods, time and location of the different environmental mechanisms are not considered, instead, these factors are calculated in generic conditions. For example, the continuous emission and infinite time for steady state condition for fate in environment, average eating habits of western Europe population for the exposure, linear approximations of the dose-effect curves, etc.

Midpoint CF_m are often calculated with respect to a reference substance ref:

$$CF_{m,s}^{final} = \frac{CF_{m,s}}{CF_{m,ref}} \quad \text{Equation II.7}$$

For example, in ReCiPe method (Goedkoop et al., 2009), 1,4-dichlorobenzene is used as reference substance for toxicity and ecotoxicity impact categories.

Endpoint characterization factors (CF_e) can also be calculated by including a damage factor DF:

$$CF_{e,s} = DF_s \times EF_s \times XF_s \times FF_s \quad \text{Equation II.8}$$

In case of human health, DF matrix represents the life years which are harmfully affected.

Climate change is one of the most evaluated impact categories. The structure of the characterization factor considered for this impact is different from the fate, effect and damage procedure applied elsewhere (Goedkoop et al., 2009). It takes into account the residence time of substances in atmosphere and their radiative forcing. The calculation of the climate change impact follows the method proposed by the Intergovernmental Panel on Climate Change (IPCC, 2013). The integrated radiative forcing of a substance was chosen as impact indicator. Till now, the calculation of the characterization factors needed a time horizon to be specified, due also to the necessity of defining some integration limits.

The radiative forcing RF_s ($W \cdot m^{-2}$) of a substance s is defined by:

$$RF_s(t) = A_s c_s(t) \quad \text{Equation II.9}$$

where A_s is the specific radiative forcing ($W \cdot m^{-2} \cdot kg^{-1}$), c_s is the time dependent concentration of s after an emission of 1 kg. The midpoint characterization factor used for climate change is the Global Warming Potential (GWP):

$$CF_{m,s} = GWP_s(TH) = \frac{\int_0^{TH} RF_s(t) dt}{\int_0^{TH} RF_{ref}(t) dt} \quad \text{Equation II.10}$$

where TH is the time horizon (year) and ref is the substance of reference, i.e. carbon dioxide.

Climate change CF is calculated for particular conditions, i.e. a pulse (Dirac) emission of the GHG and ref substance, a fixed TH for integration.

We gave in this subsection two examples of impact assessment principles, i.e. toxicity and climate change, other impact categories being addressed by similar approaches either in steady state conditions (like in toxicity method) or using a pulse emissions and a finite time horizon (like in climate change method).

1.2.4. Interpretation step

Commonly a LCA study is dedicated to the comparison of scenarios fulfilling the same function, and/or to the comparative analysis of the constituent parts of a product system. Some aspects can be raised or performed during the interpretation of a LCA study: consistency and completeness check; contribution and perturbation analysis; uncertainty and sensitivity analysis; conclusions and recommendations (Guinée et al., 2002).

1.2.5. Some limitations of the LCA method

Reap et al. (2008) discussed several limitation of the current state of LCA. They pointed out some weaknesses such as data quality, allocation, uncertainty, temporal and location consideration, allocation etc. The temporal aspect, directly related to the thesis subject, is discussed here.

The production systems the inventory step attempts to describe are highly dynamic and their behaviour depends on different temporal aspects. However, temporal information is not considered in this step:

- all datasets in LCA databases are quantities and not flows;
- the emissions and resources are represented by values without a time location;
- the intermediate flows of the technological matrix are not scheduled in time.

In traditional LCA, the mass of the emitted substance is linked to the impact by using characterization factors as proportionality constants, even though the combination of substance fate, exposure and effect phenomena are time-dependent and non-linear.

An infinite time horizon and continuous emission for steady-state condition is generally used for the calculation of CF for toxicity impact. This assumption is important for taking all long lasting impacts into account. However, predicting impacts for eternity is also illogical. Also, the consideration of an infinite time horizon may hide the potential impacts occurring over short periods of time in the

assessment of a system, because of the different nature of substances considered in the assessment (Huijbregts et al., 2001).

For other impact categories e.g. climate change, CF are calculated in the condition of a pulse emission (at time zero) and a fixed time horizon is used. It is thus legitimate to question the soundness of that method.

I.3. Temporal consideration in LCA

Only recently several research teams addressed the temporal aspect in LCA method. We distinguish between works in the field of LCI and in the field of LCIA. Here below, a brief bibliographic revue is presented concerning the development of dynamic methods within LCA. The bibliography was more specifically treated in dedicated chapters following the subject analysed.

We stress here that temporal variations in the field of technological development, economic strategies, and changes in products or value chains are beyond the scope of the thesis. These topics are addressed commonly by distinct scenario variants with attributional LCA or by consequential LCA.

I.3.1. Dynamic Life Cycle Inventory

Temporal information in the LCI step have been considered as being part of the uncertainty and using probabilistic scenario analysis (see e.g. Huijbregts 1998; Huijbregts et al. 2001). The issue with this approach is that the temporal variability is aggregated with other sources of uncertainty.

Some studies considered the distribution of emissions over time (Collinge et al. 2013; Kendall et al. 2009; Pehnt 2006; Stasinopoulos et al. 2012; Zhai and Williams 2010) in limited parts of the production system, mostly for the foreground process. Considering time dimension in every level of the production chain would be an almost impossible task without a clearly defined methodology and dedicated computational tools.

Collet et al. (2014) proposed to consider the time dimension only for selected economic/environmental flows based on their influence on the impact values. Time scales were qualitatively attributed to impact categories and inventory flows. The authors defined a perturbation factor based on the sensitivity analysis of impact results on the variation of economic/environmental flows. The perturbation factor was used to identify the combination process-economic flow-impact for deserving a dynamic study. However, a dynamic approach was proposed for neither LCI nor LCIA.

Beloin-Saint-Pierre et al. (2014) developed an approach called Enhanced Structure Path Analysis, in which environmental interventions (elementary flows, i.e. emissions and natural resources consumed)

are distributed over time by considering the convolution product between temporal distributions related to the products demand and temporal distributions related to elementary flows. This method has the merit to be the first attempt of modelling a dynamic LCI; however it still lacks important parameters for describing the process network and a full and complete relationship with an LCA database.

In the global context of DyPLCA project, Tiruta-Barna et al. (2016) have provided a dynamic method for LCI, dealing with the complex supply chain and processes involved in the life cycle system, and linking the method to traditional LCA tools and databases. At full-term of development the method will enable easier implementation of temporal characteristics by LCA practitioners.

1.3.2. Dynamic Life Cycle Impact Assessment

In the field of LCIA, climate change is the most studied impact category for the consideration of the time dimension. The first attempt to alleviate the inconsistency of a fixed time horizon was the proposition of CF for 20, 100 and 500 years – this is what actually LCA databases offer yet.

Cherubini et al. (2011) applied a dynamic method which considers a dynamic carbon removal by biomass. Their method is based on radiative forcing parameter. They combined a function of carbon dioxide decay in atmosphere and the carbon uptake given by a rate of biomass growth. However, dynamic results for midpoint or endpoint climate change impact are not given as the calculated results are integrated in a single unit-based index. Also, only carbon dioxide was assessed and other substances that contribute to climate change were neglected.

Levasseur et al. (2010) and Kendall (2012) studied time dependency in climate change impact by calculating temporal characterization factors (CF) based on radiative forcing indicator. These CF were calculated for 1 year interval and were applied to a case study with a simple dynamic emission. This method still conserves the main principle of conventional LCA, i.e. the CF utilization and the time horizon concept. Nonetheless, thousands of CF values must be calculated for few substances and a limited time horizon, which makes the method heavy to apply.

In case of toxicity impact category, CFs for 20, 100 and 500 years were calculated to be in accordance with the time horizons used for GWP, as it was considered that they provided a useful interval for policy decisions. Those CFs were calculated with USES-LCA model for CML LCIA method (Huijbregts et al., 2000a, 2000b, 2001).

Similarly to the method of Levasseur for climate change, Lebailly et al. (2014) proposed to calculate CFs for substances for every 1 year passed after the initial emission. In this aim, the authors used the USEtox[®] model for a pulse, unit load of substance by solving the fate model for these particular

conditions. Then they applied the method to a case study – the use of zinc as fertilizer in agriculture. Moreover, the case study did not address the behaviour of non-persistent substances (organics) and did not implement complex, temporal LCIs, as actually occur in real LCA case studies. Here again, as in case of climate change, the main principles and, at the same time limitations, of conventional LCA are present, i.e. preservation of the ‘characterization factor’ concept, a particular calculation condition (pulse emission) and time horizon.

I.4. Research objectives

LCA method is widely used for the evaluation of environmental consequences of anthropogenic activity. Among the limitations of LCA, the consideration of temporal dimension was little addressed and few developments were proposed so far.

Temporal characteristics are essential to describe the non-steady state profile of complex processes and supply chains. The dynamic characteristics of the environmental interventions produced by a product system depend on the nature of those activities, supply chain, stock of goods, seasonality, time lags, etc. The impact generation in nature caused by anthropogenic emissions is also dynamic. Climate change, ozone depletion, acidification, human and ecotoxicity are few examples of impacts that depend on the concentration of concerning substances in environmental compartments. Environmental mechanisms involved in impact generation also have their own temporal behaviour depending on multiple bio-, physical and chemical phenomena such as mass and heat transfer, chemical and biological reactions, food chains, etc. Until now, few researches were dedicated to the development of models and methods for the time integration in LCA. They usually concerned only one aspect of the dynamic features in one LCA step at a time.

The research work presented in this PhD thesis is part of a major project called DyPLCA (Dynamic Processes Life Cycle Assessment) which is funded by the French national research agency (ANR) and the Luxembourg national research agency (FNR).

The global objective of the project is the development of an operational method and associated tools (software) for dynamic LCA.

Given the different axis for the development of a complete dynamic LCA framework, different fields of expertise are necessary for the proper development of the project. For this reason, different institutions contribute to DyPLCA project:

- Laboratoire d'Ingénierie des Systèmes Biologiques et des Procédés (LISBP): located in the National Institute of Applied Sciences (INSA Toulouse), this institute brings expertise in process modelling (chemical/biochemical processes) and LCA.
- Luxembourg Institute of Science and Technology (LIST): recognized expertise in many axes of LCA.
- Université du Havre, Laboratoire d'Informatique, du Traitement de l'Information et des Systèmes (LITIS): this partner offers expertise in informatics more specifically in the development of graph based algorithms and visualization.
- Centre Scientifique et Technique du Bâtiment (CSTB): expertise in the field of buildings.

In this context,

The major objective of this study is to contribute to the development of a complete framework for dynamic LCA:

- 1. Development of dynamic models and tools for the LCIA step, more precisely for climate change and toxicity impact categories;**
- 2. Contribution to the integration of temporal features in the LCI step.**

1.4.1. Thesis outline

This thesis report is structured in 6 chapters.

Chapter I (this chapter) introduces the background concerning conventional and dynamic LCA. In this context, the research objectives and the corresponding tasks are defined.

Chapter II describes the adaptation performed on a LCA database in order to include temporal parameters for the calculation of LCI. The methodology for defining temporal parameters for chemical/biochemical processes and waste treatment processes was explained.

Chapter III presents the method proposed for the time consideration in the calculation of climate change impact. Two different indicators were analysed: global mean temperature change and radiative forcing. Additionally, the dynamic climate change method was applied in a case study (production of bioenergy from microalgae) for demonstrating its feasibility.

Chapter IV presents the method proposed for the temporal consideration in the calculation of toxicity/ecotoxicity impacts. The method proposed is based on the USEtox[®] model and Simplebox

model for dynamic fate calculation. A case study was performed (production of grapes) allowing highlighting the features of the new method.

Chapter V presents the complete framework developed for the calculation of a dynamic LCA and the application to a case study. Moreover, a sensitivity analysis was performed aiming at evaluating the influence of the detail level of LCI time definition (time granulometry) on the dynamic impact results.

Lastly, chapter VI presents the conclusion and the main findings of this work as well as perspectives following this thesis.

Additionally, supplementary information is provided in annexes concerning the adaptation of methods in order to include temporal parameters. The documentation for the calculation code developed for the dynamic impact calculation is also presented. Moreover, additional information and specific data for the case studies are supplied.

Note to the reader: The content of this thesis manuscript is based in either accepted or “in preparation” peer-reviewed articles. Original papers are presented in the chapters III, IV and V. The reader will find detailed literature information concerning each subject in the following chapters.

**Chapter II. Dynamic Life Cycle
Inventory: temporal database
for dynamic processes**

“Pollution is nothing but the resources we are not harvesting. We allow them to disperse because we've been ignorant of their value.”

R. Buckminster Fuller

Life Cycle Inventory (LCI) is the step in Life Cycle Assessment (LCA) where natural interventions of one production system are accounted (ISO 14040:2006, 2006). In this step, all outputs and inputs of the production system are detailed, taking into account raw resources or materials, energy, water, emissions to different environmental compartments and land use.

The production systems the inventory step in LCA attempts to describe are highly dynamic and their behaviour depends on different temporal aspects. The aggregation of emissions in a single value leads to a loss of most of the temporal features in LCI and may hide important information for the LCA practitioners. The dynamics of a production system can be related to the two main components: processes and supply-chain.

Tiruta-Barna et al. (2016) proposed a method in which temporal features of the production activities and the supply-chain are taken into account. This method uses the principle of function and reference unit (proportionality of environmental interventions quantities with the value of the reference flow) from conventional LCA method, as well as the structure of LCA databases, i.e. the technological matrix and environmental interventions matrix. Moreover, ecoinvent data base is used in the new dynamic approach. Besides, the dynamic model is linked to a ‘temporal database’ containing a set of temporal parameters defined for every process from ecoinvent. These features facilitate the use of the conventional LCA assets.

The objective of this chapter is to provide support for the development of the temporal database for the dynamic inventory method. Temporal parameters for chemical, biochemical and waste treatment processes were established. Also, possible exceptions to the proposed model were pointed out in order to achieve better dynamic characterization of specific processes.

Résumé

L'inventaire du cycle de vie (ICV) est l'étape de l'analyse du cycle de vie (ACV) où les flux élémentaires d'un système de production sont comptabilisés (ISO 14040: 2006, 2006). Dans cette étape, tous les flux de sortie et d'entrée du système de production sont détaillés, en tenant compte des ressources naturelles et les matériaux, l'énergie, l'eau, les émissions dans différents compartiments environnementaux et de l'utilisation des terres.

Les systèmes de production que l'étape d'inventaire de l'ACV décrit ont un caractère dynamique et leur comportement dépend de différents paramètres temporels. Cette dynamique peut avoir une influence significative sur le résultat de certaines études ACV (Field et al., 2000; Finnveden et al., 2009; Owens 1997; Reap et al., 2008, Udo de Haes et al., 2002). L'agrégation des émissions en une seule valeur entraîne une perte de la plupart des caractéristiques temporelles dans l'étape d'ICV et peut cacher des informations importantes. Par conséquent, les caractéristiques temporelles de l'étape d'ICV ont été considérées comme faisant partie des incertitudes de l'étude (Huijbregts et al., 2001). Cependant, la présence d'autres sources d'incertitudes peut empêcher une bonne interprétation des aspects dynamiques d'une étude.

Tiruta-Barna et al. (2016) ont développé une méthode pour le calcul de l'ICV dynamique qui considère la complexité d'une chaîne d'approvisionnement, en tenant compte du décalage entre les procédés constituant le système de produit du cycle de vie. Le développement d'une base de données temporelle pour les procédés d'arrière-plan est également prévu par leur méthode. La liaison entre la méthode d'inventaire dynamique et les outils d'ACV traditionnelle est également une caractéristique importante de la nouvelle approche.

Les objectifs de ce chapitre sont de contribuer à la construction de la base de données temporelles établissant des valeurs pour les procédés chimiques, biochimiques et de traitement des déchets et d'identifier les possibles exceptions dans le modèle proposé par Tiruta-Barna et al. (2016).

Pour créer le réseau de procédés du cycle de vie et pour placer les procédés sur une échelle de temps, un algorithme de recherche sur une structure de graphe (Breadth First Search) a été implémenté dans l'outil de calcul de l'ICV dynamique nommé DyPLCA. En ce qui concerne la représentation de graphe du réseau d'un système ACV, les nœuds représentent les activités (procédés) et les arcs représentent les flux de produits ou de services entre les procédés. Il permet la reconnaissance de l'association producteur-consommateur dans le réseau d'ACV permettant la mise en œuvre de modèles de procédés et d'approvisionnement.

Afin d'exécuter un calcul d'inventaire dynamique complet avec le modèle DyPLCA, une base de données avec les paramètres temporels pour les procédés d'arrière-plan a été développée. De plus, la base de données ecoinvent (version3.2) a été choisie pour être utilisée dans le modèle DyPLCA car

elle fournit un grand nombre de sets de données et elle est largement utilisée par les praticiens d'ACV.

L'ecoinvent 3.2 compte plus de 12 000 activités pour les produits de référence. Alors, les caractériser individuellement est presque une tâche impossible à réaliser dans un laps de temps limité. Afin de simplifier la caractérisation de la base de données, l'ensemble de données ecoinvent a été divisé en différents groupes. La classification internationale standard des activités industrielles et économiques (ISIC) a été utilisée comme méthode de classification dans la base de données temporelles (Nations Unies, 2008). La révision 4 de la classification ISIC comprend 4 niveaux: section, division, groupe et classe. Par conséquent, le niveau « classe » a été utilisé pour la tâche de caractérisation temporelle des activités. Le travail de construction de cette base de données temporelles a été partagé entre les partenaires du projet DyPLCA selon leur domaine d'expertise.

Le laboratoire LISBP a été chargé de caractériser les processus de traitement des déchets et eaux usées et la fabrication de produits chimiques. Afin de caractériser les paramètres temporels de ces procédés, la base des données ecoinvent a également été analysée, ainsi que la documentation existante pour ses ensembles de données. Lorsqu'aucune donnée n'a été retrouvée dans les documents ecoinvent, les ressources externes ont été analysées. Même si une division a été effectuée pour diminuer la quantité de sets de données analysés par chaque groupe de travail, la quantité de données à caractériser était encore importante. À cet égard, des sets de données arbitraires ont été choisis afin d'identifier leurs paramètres temporels. Les mêmes valeurs des paramètres temporels ont été ensuite attribuées au groupe entier de l'ISIC une fois que l'analyse d'un grand nombre de sets de données du même groupe indiquait qu'elles s'appliquent pour la plupart des procédés. Certains procédés ont été identifiés comme des exceptions car leurs paramètres temporels ne correspondent pas à ceux du groupe ISIC.

II.1. Introduction

Life cycle inventory (LCI) is the step in life cycle assessment (LCA) where natural interventions of one production system are accounted (ISO 14040:2006, 2006). In this step, all output and input flows of the production system are detailed, taking into account raw resources or materials, energy, water, emissions to different environmental compartments and land use.

Nevertheless, the production systems the inventory step in LCA attempt to describe are highly dynamic and their behaviour depends on different temporal aspects. These dynamics might have significant influence in the outcome of certain LCA studies (Field et al. 2000; Finnveden et al. 2009; Owens 1997; Reap et al. 2008; Udo de Haes et al. 2002). The aggregation of emissions in a single value leads to a loss of most of the temporal features in LCI and may hide important information for the LCA practitioners. Therefore, temporal characteristics in LCI have been considered as part of the uncertainty of the study (Huijbregts et al. 2001). However, the presence of other sources of uncertainty may not allow a proper interpretation of a dynamic study.

Several authors already modelled their processes in order to include temporal information in particular case studies. For example Collinge et al. (2013) and Pehnt (2006) modelled the studied processes by taking account of several temporal characteristics such as process operations, supply chain dynamics, etc. Nevertheless, it is not clear how that modelling was performed and what temporal variables they considered. Moreover, a dynamic LCA methodology requires a general framework with operational tools for temporal LCI building.

Beloin-Saint-Pierre et al. (2014) developed an approach called Enhanced Structure Path Analysis, in which environmental interventions (elementary flows, i.e. emissions and natural resources consumed) are distributed over time by considering the convolution product between temporal distributions related to the process flows (intermediate flows) and temporal distributions related to elementary flows. However, this method still lacks the fully and complete relationship with a LCA database which is essential for the consideration of time for the background processes. Moreover, the temporal characteristics of the supply chain are not taken into account in their method.

The importance of lag time consideration in the supply chain of a production system in LCA is highlighted by Collinge et al. (2013). They draw special attention to the fact that a complete formulation of a supply chain would require the use of a network structure because the number of time lags would substantially increase for each level back through the supply chain.

Tiruta-Barna et al. (2016) have provided a dynamic model for LCI, considering the complex supply chain and temporal behaviour of processes. This new approach reuses traditional LCA databases

(ecoinvent for instance) coupled with a new temporal data base. The temporal database is under development and includes temporal parameters for processes and supply chains. Linking the dynamic model to the traditional LCA tools is also an important asset of the new method.

The objectives of this chapter is to contribute to the development of the temporal data base by establishing temporal parameters for chemical, biochemical and wastewater processes and by identifying possible datasets exceptions with respect to the model proposed by Tiruta-Barna et al. (2016).

II.2. Method

In this section a brief description of the dynamic LCI model and temporal data base principles are provided.

II.2.1. Temporal LCI model and DyPLCA tool

An extended description of the temporal LCI model is presented in Tiruta-Barna et al. (2016); only the main principles are recalled below.

LCA conventional method and databases provide a technological (A) matrix and an environmental intervention (B) matrix. After setting a functional unit, the scaling (S) vector is calculated (as shown in Introduction chapter). Technological matrix provides the network of the process system as the non-diagonal values indicate the quantitative relationships between processes.

The temporal LCI model is based on the conventional inventory (matrixes A and B) and on a few temporal parameters and functions. Process dynamics is represented by the functions alpha and beta and the parameters r , T , t_0 , all defined in Table II.1 and Figure II.1. Supply function φ is defined through δ and τ parameters.

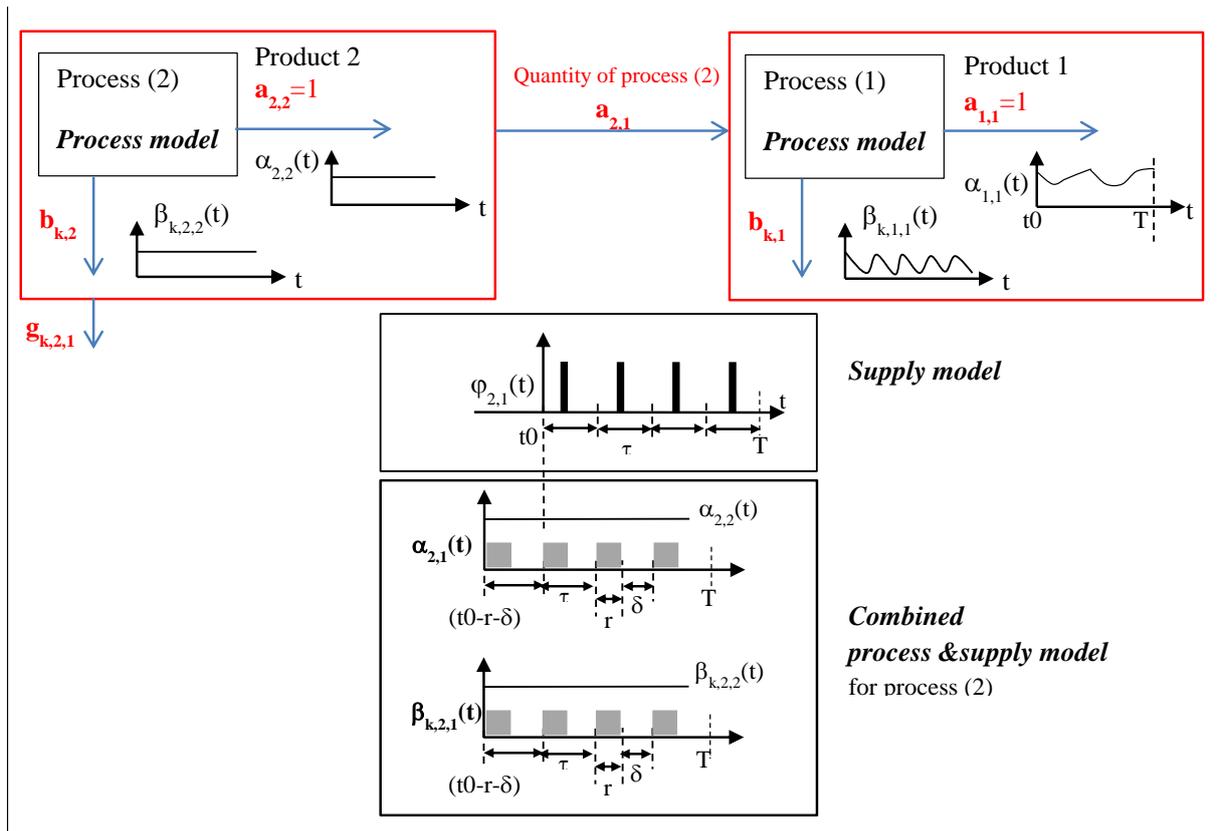


Figure II.1 – Two subsequent processes: current ecoinvent related data (in red); process model, supply model and their combination. Legend for variables: a_{ij} and b_{kj} : elements of matrix A and B (i, j are processes, k is an environmental intervention); α_{ii} and β_{kii} : production and emission functions for process i ; T : functioning period for the system; t_0 : evaluation's start time; δ : supply delay period; r : production period; τ : period of supply of product 2 for process 1; $\varphi_{2,1}$: supply function from 2 to 1; $\alpha_{2,1}$ and $\beta_{k,2,1}$: production and emission functions for process 2 working for process 1; $g_{k,2,1}$: quantity of k emitted by process 2 when working for process 1. From Tiruta-Barna et al. (2016).

Table II.1 – Parameters for time consideration in the DyPLCA model

	Parameter	Name	Significance
Process model (specific for process i)	$\alpha(t)$	Production function	Describes the time shape of the activity (e.g. continuous, constant, discontinuous...)
	$\beta(t)$	Environmental intervention function	Describe the time shape of the emissions/resource consumptions. Usually linked to $\alpha(t)$
	r	Production period	Time between the earliest input (raw material) and the latest output of the activity
	T	Representative period	Life time of the main infrastructure (material support) related to the activity
	t_0	Start date of the analysis	Arbitrary or calendar dependent
Supply model (process link i-j)	δ	Delay	Storage time, no activity takes place
	τ	Supply period	Supply frequency for intermittent supply; $\tau=T$ for continuous supply
	$\varphi(t)$	Supply function	Continuous or intermittent supply

The normalized functions alpha and beta link the conventional inventory to the temporal model in the sense that the integral of these functions over the defined life time T of the process results in the inventory data $a_{i,i}$ in technological matrix A and $b_{s,i}$ in intervention matrix B (Equation II.1 and Equation II.2).

$$a_{l,l} = \int_{t_0}^{t_0+T} \alpha_{l,l}(t) dt \quad \text{Equation II.1}$$

$$b_{s,l} = \int_{t_0}^{t_0+T} \beta_{s,l,l}(t) dt \quad \text{Equation II.2}$$

where $\alpha(t)$ is a flow of material, energy or service and is represented by the reference unit by time (e.g. $\text{kg}\cdot\text{h}^{-1}$, $\text{m}^3\cdot\text{day}^{-1}$, $\text{kWh}\cdot\text{s}^{-1}$, etc.), $\beta(t)$ is the flow of the environmental intervention s ($\text{unit}\cdot\text{time}^{-1}$), l is the level on the supply chain and s is the substance.

Every activity in the process flow presents its own start date (t_0) which can be expressed by:

$$t_0^{l+1} = t_0^l - r - \delta \quad \text{Equation II.3}$$

where r represents the production period and δ represents the lag period. The parameter t_0 is applied for both production and environmental intervention functions and represents the key parameter for the distribution in time of the environmental interventions over the life cycle time span of a system.

The supply chain model describes the schedule and quantity delivered of a producer process to a consumer (Equation II.4). The integral of the supply function is the non-diagonal value $a_{i,j}$ of the technological matrix A , which describes the quantity needed of a certain process j by process i :

$$a_{l+1,l} = \int_{t_0}^{t_0+T} \varphi_{l+1,l}(t) dt \quad \text{Equation II.4}$$

The combination of Equation II.1, Equation II.2, Equation II.3 and Equation II.4 leads to the calculation of the intermediary flows between processes (Equation II.5) and environmental interventions flows (Equation II.6).

$$\alpha_{l+1,l}(t) = -\frac{s_l a_{l+1,l}}{C_{l+1}} \alpha_{l+1,l+1}(t) dt \quad \text{Equation II.5}$$

$$\beta_{s,l+1,l}(t) = -\frac{s_l a_{l+1,l}}{C_{l+1}} \beta_{s,l+1,l+1}(t) dt \quad \text{Equation II.6}$$

The term $s_l a_{l+1,l}$ represents the quantity of the reference flow $l+1$ delivered by process $l+1$ towards process l . C represents a production capacity parameter

$$C_{l+1} = \frac{T_l}{\tau_{l+1,l}} \int_t^{t+r_{l+1}} \alpha_{l+1,l+1}(t) dt \quad \text{Equation II.7}$$

The final objective of the model is to obtain the environmental interventions distributed in time, i.e. all beta functions. Their integration over time (between initial i and final f time values) retrieves the conventional inventory results, i.e. $g_{s,l+1,l}$ quantities for each substance s and each process $l+1$ linked to process l (see Chapter I).

$$g_{s,l+1,l} = \int_{t_{0_i}}^{t_{0_f}+T_f} \beta_{s,l+1,l}(t) dt \quad \text{Equation II.8}$$

Then, these functions can be summed for a given substance s , in order to obtain the $\gamma(t)$ functions, or the aggregated inventory g_s for that substance.

To create the supply chain network and emplace the processes on the time scale (i.e. t_0 for every process), a graph search algorithm, namely “breadth first search”, was implemented. In the graph representation of the LCA system network, the nodes represent the processes and the bridges represent the product or services flows between the processes. It allows the recognition of the relationship consumer-producer in the process network enabling the implementation of the process and supply quantitative models.

The tool developed, DyPLCA, is available at <http://dypclca.univ-lehavre.fr/>. For a given case study, the conventional matrixes A and B are imported in order to retrieve the values $a_{i,j}$ and $b_{s,i}$. By now, the DyPLCA is only adapted for the matrix results from Simapro[®] v8 software and it is not compatible yet with other LCA software. The temporal data base is used for the temporal parameters of the background processes. The foreground processes can be defined (processes, links and temporal parameters) on the DyPLCA interface. Following strictly the term “cradle to grave” would imply massive computational time for the calculation of the dynamic inventory. For this reason, a threshold for the mass flow and a time limit backwards are imposed for the dynamic LCI calculation.

DyPLCA tool was developed in two stages. The first version of the DyPLCA tool allowed the modelling of the process network on the web platform but there were no integration with a temporal database. The second version presents the described functionalities, i.e. import of conventional A and B matrixes, use of a temporal data base for the background processes and definition of the foreground processes on the web interface.

II.2.2. Development of a temporal database

In order to perform a complete dynamic inventory with DyPLCA model, a database with the temporal parameters for the background processes was planned to be developed. Ecoinvent database were chosen for use in the DyPLCA model as it provides a wide variety of datasets and it is widely used by LCA practitioners. The temporal data base should complete ecoinvent with temporal information for every process. The task consisted in the collection and definition of the temporal parameters and functions listed in Table II.1 (except t_0) for all reference products. These parameters are collected in an Excel file with, in rows the reference products and in columns the model parameters.

Ecoinvent database 3.2 has more than 12 thousands activities for reference products. Characterize them individually is almost an impossible task in a limited period of time. In order to simplify that task, ecoinvent datasets were classified in different groups. The International Standard Industrial Classification of All Economic Activities (ISIC) was used as the method of classification of the datasets (United Nations, 2008). The version 4 of the ISIC classification contains 4 levels: section, division, group and class. Therefore, the class level was used for the task of temporal characterization of the database, task which was divided between different working groups in DyPLCA project. The division was made in order to respect the field of expertise of each working group. LISBP laboratory was responsible for characterizing the processes describing the manufacturing of chemical products, waste treatment. LIST partner was in charge of all the others datasets and the compilation in the final form.

II.3. Results and discussions

A part of the temporal data base was built in this work and the main results are presented below. During the database development, we observed that the general model for the dynamic LCI calculation do not comply with some activities in ecoinvent 3.2. Consequently, modifications of the model were proposed case by case and several were already implemented.

II.3.1. Database adaptation for chemical and bio-processes

The ISIC groups which were designated to LISBP laboratory were mainly related to chemical industries and waste treatment processes. In order to characterize the temporal parameters of these processes, ecoinvent was analysed as well the reports available for its datasets. When no data was retrieved in the ecoinvent documents, external resources were analysed. Even though a division was done to diminish the quantity of datasets analysed by each working group, the amount of data to characterize was still important. Consequently, arbitrary datasets were chosen in order to identify the temporal parameters of the different ISIC groups. The same values of temporal parameters were then attributed to an entire ISIC group once the analysis of a great number of datasets indicated that they applied for most of processes. Some processes were cited as exceptions as their temporal parameters do not correspond to the ones of the ISIC group and they will be described in dedicated sections. Finally, even though efforts to meticulously analyse the database were done, some processes which were attributed the general ISIC group temporal parameters may be part of exceptions and vice-versa.

In the following, only one category of reference products is presented. For sake of simplicity, all other categories investigated are presented in annex (SI I). The same work methodology was applied.

II.3.1.1. Manufacture of basic chemicals

Ecoinvent database presents 1224 activities which are included in the ISIC group “Manufacture of basic chemicals”. The activity “Chemical plant, organics” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period (T) parameter is based in the infrastructure lifetime of “Chemical plant, organics” activity. The value presented in this dataset is 50 years and the same value is also applied for land use (Althaus et al, 2007).

The value for the parameter delta was chosen as the “consensus” of different datasets. “Methanol from natural gas” and “Methyl chloride / Tetrachloroethylene, at regional storage” are some of the processes which showed a value of 2 months for storage of products before shipping (Althaus et al, 2007). For solid chemicals, the storage time is also considered 2 months as described in the section “Storage building, chemicals, solid” of Althaus et al, (2007). Therefore, the value of 2 months is then considered as delta for the ISIC group “Manufacture of basic chemicals”.

The production time in a chemical process can last between hours to days because it depends on the time required for the downstream, the upstream, the time of reaction, etc. For this ISIC group, the general value assumed for the parameter r was 1 day as chemicals processes do not usually last long.

The function alpha was considered as constant value of $0.02 \text{ kg}\cdot\text{year}^{-1}$ (i.e. 1 kg/50 years) As the emissions from a process are linked to the process functioning, the beta function was also considered as a constant: it was calculated by the product between the same constant value and the value of b element in the intervention matrix B for the respective substance. The constant value means that the production and the associated emissions are steady during the production period r.

Exceptions

Hereafter, six different activities are described as exceptions (processes that do not present the same general temporal characteristics): “methanol production”, “air separation, xenon krypton purification”, “air separation, cryogenic”, “citric acid production”, “Chemical production, inorganic”, “chemical production, organic” and activities which mention in their names “... to generic market...”. The temporal parameters which are not cited as exceptions are then the same as those of the ISIC group.

The activity “methanol production” has a particular process of infrastructure which is called “Methanol plant” (Althaus et al, 2007). The difference between this dataset and parameters considered for the ISIC group is the representative period T. The value of infrastructure lifetime presented in the dataset “Methanol plant” is 30 years.

The activities “air separation, xenon krypton purification” and “air separation, cryogenic” present a particular process for infrastructure which is called “air separation facility”. The parameter for the representative period of these processes is considered as 20 years (Althaus et al, 2007).

The dataset “citric acid production” has citric acid as product which is mainly made from a fermentation reaction. Anastassiadis et al. (2001) considers the retention time of the reaction between 60 and 120h. For this reason, the parameter of production period r was considered as 5 day.

“Chemical production, inorganic” and “chemical production, organic” activities present an unweighted average of the first 20 substances which are part of the top100 chemicals included in ecoinvent 3.2 database. For this reason, no temporal parameters were designated for this activity.

Activities which mention “... to generic market...” (e.g. “acetonitrile to generic market for solvent for chromatography analysis” and “tin dioxide to generic market for polishing powder”) do not have the same temporal characteristics as the ISIC group “Manufacture of basic chemicals” processes. Those activities have the purpose to link some processes to markets. There are no emissions or other activities presented in this dataset. Therefore, it is considered that the dataset does not have any temporal characteristics.

II.3.2. Exceptions in DyPLCA model

The method presented by Tiruta-Barna et al (2016) is suitable for the dynamic calculation of material and energy production processes. Some basic principles are considered by the model presented until now:

- The producer process always takes place before or at the same time as the consumer process
- The product from a process can be delivered in batches with a constant periodicity defined by the parameter τ .
- Energy (heat and electricity) is produced and distributed continuously and the supply/delivery will have the same duration as the representative period of the consumer activity.

However, after analysing the data sets we observed that some processes do not follow all these assumptions. They can be categorized in five distinct groups:

- Markets
- Services
- Recycling
- Infrastructure
- Imposed date processes

These drawbacks, presented hereafter, are currently being taken into account and new features are (or will be) soon available in the DyPLCA model. The current version of the temporal data base discriminates the activities considered as “markets” inecoinvent 3.2, and also activities considered as “services”. Those activities belonging to these categories are flagged in the temporal data bases.

Markets

Markets are a particular definition of an activity which concerns a general group of the same reference production in a specific geography. It also might include transports of the reference product. The market activity is not a production process or a service, for this reason, market activities does not present any temporal characteristics. The market activity is by-passed during the graph search algorithm. This feature is already included in the DyPLCA tool.

Services

Material and energy production processes take place in time before the utilization of their products by the consumer process. They have to be produced and they have to be ready for delivery prior to the initial time of the consumer process. However, this time scheduling is not valid for services. The acquisition of a service by a consumer process usually happens at the same time or later than the activity of the consumer process. For example, in the case of an agricultural system, the process of watering has to take place during the production period of the agricultural process. Another example, the treatment activity of the waste produced by a plant takes place at the same time as the plant functioning and not prior to that.

When considering the calculation of t_0 (i.e. the position of alpha and beta functions in time) of a certain process, the general assumption is that the batch of the producer which will supply the consumer activity starts and finishes before the acquisition by consumer activity. However, in the case of a service activity, the t_0 of the process must happen after or at the same initial time of the consumer activity as its functioning occurs during the production period of the consumer activity. In this sense, the t_0 of the service process (producer) could be set to t_0 of the consumer.

This specific case was implemented in DyPLCA model.

Recycling

The reasoning for this category is almost the same as for the service category. The functioning period of the recycling process would occur only after the production period of the recycled material, i.e. the producer process. Initial time of a recycling process have to happen only after the end of the production of the material. The initial time t_0 of a recycling activity could be calculated as the sum of the t_0 , r and δ of the consumer.

This modification was not implemented in DyPLCA tool.

Infrastructure

Infrastructure is a particular case of material production, e.g. construction of a plant infrastructure. It will happen only once in the plant lifetime or more generally in the lifetime of an activity.

The activities identified as infrastructure does not follow the same rules for the calculation of the production capacity parameter. This case is more complex and was not yet investigated.

Imposed date

The general calculation of t_0 of a producer process depends on parameters r , δ and t_0 of the consumer process (Equation II.3). Following these criteria, the initial time of the process might happen anywhere on the time scale (in the sense of calendar time). For some specific processes, the calculation of t_0 does not apply as they must be placed in a specific period on the calendar. For example, agricultural processes have usually a specific date in which their products are sown, grown and harvested. For this reason, a specific temporal parameter which indicates a specific start date has to be implemented.

II.4. Conclusions

The new approach allows the proper consideration of the dynamic features of a huge network of processes for the LCI temporal modelling. Supply chain consideration with simple temporal parameters allows an efficient calculation of emissions over time without neglecting all the dynamic characteristics of a production system. However, this method still needs the implementation of other features in order to consider all categories of processes which are presented in ecoinvent database. Therefore, updates and new implementations are already expected in the DyPLCA tool which may alleviate these limitations.

The data collection for the creation of the temporal database is a great step forward in the development of a fully operational tool for dynamic LCA. The division of the database processes in the categories proposed by the ISIC classification allowed the task to be feasible. The same temporal parameters may

be attributed to activities belonging to the same ISIC category. Nevertheless, activities which do not follow the general assumptions within a specific ISIC group were also considered and were treated specifically.

More specifically, this study attributed temporal data for chemical processes and waste treatment activities existent in ecoinvent 3.2 database. Moreover, a deep analysis of ecoinvent processes allowed propositions for the improvement of the general dynamic LCI model. Several of them have already been implemented in DyPLCA tool.

Further development of the temporal database is envisaged in order to increase the accuracy of the attributed temporal data. From now on, the attribution of temporal data in ecoinvent database from contributors would be of great importance for the development of the dynamic LCA method.

Chapter III. A dynamic approach for Climate Change impact

“As human beings, we are vulnerable to confusing the unprecedented with the improbable. In our everyday experience, if something has never happened before, we are generally safe in assuming it is not going to happen in the future, but the exceptions can kill you and climate change is one of those exceptions.”

Al Gore

The climate disturbance is at the present undeniable. Changes that have been observed since 1950s are unprecedented over decades to millennia. The effect can be seen such as the warming of atmosphere and ocean, amount of snow and ice has decreased, sea level increased as well the concentration of greenhouse gases (IPCC, 2013). Radiative forcing increased 2.29 W.m^{-2} between 1750 and 2011. Its increasing rate is more important than in the prior decades (IPCC, 2013). Climate change is therefore an important impact to be analysed in a LCA study.

The present chapter aims to provide a dynamic method for the dynamic assessment of climate change impact. Two indicators were proposed: global mean temperature change and radiative forcing. The developed dynamic climate change methods can be applied to any kind of GHG temporal emission whatever its temporal profile. No characterization factors are provided, instead, climate change indicators are calculated in function of time. A Python program was developed for the dynamic climate change calculation and its interconnection with the DyPLCA inventory.

The case study presented in this chapter is published in the “Journal of Cleaner Production”, 139 (51-60) doi: 10.1016/j.jclepro.2016.08.003. It concerns the production of bioenergy from microalgae as potential alternative raw material. Different technologies were proposed for the transformation of the algal biomass into energy products. In this study, two bioenergy production systems were modelled and their environmental efficiency was assessed: a biodiesel system and a biogas system. Dynamic Life Cycle Assessment (DLCA) is used to demonstrate the possible existence of carbon sequestration by microalgae and to analyse the temporal characteristics of the production system.

Résumé

Le réchauffement climatique est désormais une évidence. Les changements observés depuis les années 1950 sont sans précédent. L'effet de l'augmentation de la concentration des gaz à effet de serre peut être observé sur le réchauffement de l'atmosphère et de l'océan, les quantités de neige et de glace ont diminué et le niveau de la mer a augmenté (IPCC, 2013). Le forçage radiatif a augmenté de $2,29 \text{ W}\cdot\text{m}^{-2}$ entre 1750 et 2011 et son taux de croissance est plus important que dans les décennies précédentes (IPCC, 2013). Le changement climatique est donc un impact important à analyser dans une étude d'ACV.

Ce chapitre vise à fournir une méthode pour l'évaluation de l'impact changement climatique en fonction du temps. Deux indicateurs ont été étudiés: la variation de la température moyenne et le forçage radiatif. La méthode proposée permet d'obtenir des informations temporelles importantes sur la réponse de l'environnement aux émissions dynamiques des gaz à effet de serre (qui viennent des résultats de l'inventaire dynamique). En ce sens, un programme Python a été développé afin d'interconnecter l'inventaire dynamique DyPLCA avec le modèle dynamique du changement climatique.

L'indicateur basé sur le forçage radiatif considère la dynamique des GES dans les compartiments environnementaux. L'indicateur basé sur le changement de température moyenne globale ajoute à l'indicateur précédent la dynamique des phénomènes thermiques de la planète. L'approche des modèles type boîte-noire a été utilisée pour le calcul des indicateurs. Les paramètres physiques qui représentent les indicateurs de réchauffement climatique ont été modélisés comme des réponses du système « environnement » à la perturbation « émission de gaz à effet de serre », en utilisant les fonctions de réponse impulsionnelle et leur produit de convolution avec les perturbations respectives.

Des caractéristiques importantes ont été mises en évidence dans cette approche: 1) une valeur maximale de la variation de température est atteinte à un certain point dans le temps en fonction du profil d'émission, qui est négligé dans la méthode conventionnelle; 2) la comparaison avec les résultats de la méthode conventionnelle a montré qu'un horizon de temps fixé est arbitraire par rapport au système étudié et peut conduire à des classements différents entre les scénarios étudiés lorsque l'horizon temporel est modifié; 3) la méthode proposée n'est pas basée sur un facteur de caractérisation pré-calculé, le calcul peut être effectué pour la durée souhaité et n'utilise pas une substance de référence.

Le cas d'étude présenté dans ce chapitre a été publié dans la revue Journal of Cleaner Production, 139 (51-60) doi: 10.1016 / j.jclepro.2016.08.003. Il s'agit de la production de bioénergie à partir de microalgues comme matière première alternative. Diverses technologies ont été proposées pour transformer la biomasse des algues en produits énergétiques. Dans cette étude, deux systèmes de

production de bioénergie ont été modélisés et évalués: un système de production de biodiesel (et ses sous-produits chaleur et électricité) et un système de production de biogaz (avec ses co-produits chaleur et électricité).

Plusieurs indicateurs ont été calculés pour l'évaluation de la production d'énergie de microalgues (biodiesel, chaleur et électricité): bilan énergétique, l'ACV et l'ACV en dynamique. Les résultats montrent que les technologies pour la production à grande échelle de bioénergie à partir de microalgues doivent encore être améliorées et optimisées pour réduire leurs impacts sur l'environnement. La production de biodiesel est très consommatrice d'énergie, principalement en raison des opérations unitaires de séchage et d'extraction des lipides en utilisant des fluides supercritiques. Les résultats globaux montrent une meilleure performance environnementale pour la technologie la plus simple, à savoir le système biogaz.

En ce qui concerne les caractéristiques temporelles des processus, l'évaluation dynamique du changement climatique a montré que la production de bioénergie à partir de microalgues ne conduit jamais à la séquestration du carbone. Les algues sont souvent la seule possibilité de valoriser les sites naturels modifiés par une activité antérieure comme l'extraction du sel marin, ou de tirer profit des étangs naturels en bord de mer. Dans ces sites, les conditions de croissance des algues peuvent être naturellement optimales, ce qui facilite une productivité élevée. La question de trouver les méthodes de transformation les plus efficaces se pose alors. Le panel de processus et de produits proposés à partir de microalgues augmente, mais aucune technologie industrielle n'est en cours de développement, à l'exception de certaines applications alimentaires. Outre les aspects économiques, l'analyse énergétique et environnementale est cruciale pour le choix d'un processus de transformation durable.

III.1. Introduction

The emissions released into air can contribute to different impacts such as climate change, ozone depletion and photochemical smog. Global warming has received special attention as the increasing in temperature was about 0.85°C (0.65°C to 1.06°C) over the period 1880 to 2012. The temperature in Northern Hemisphere was the warmest in the period between 1983 and 2012 in the last 1400 years (IPCC, 2013). Considering contributing gas species to global warming, carbon dioxide, methane and dinitrogen monoxide are the main greenhouse gases (GHG) released in atmosphere (IPCC, 2013).

Global Warming Potential (GWP) is the metric adopted by the most of Life Cycle Assessment (LCA) practitioners for the calculation of climate change impact category (Levasseur et al. 2010). GWP represents the relative value of the cumulative radiative forcing resulting from a unitary impulse emission of certain substance by the result of carbon dioxide (in the same conditions). The atmospheric load of CO₂ after an emission is predicted by climate models, such as the Bern carbon cycle-climate model, which are based in carbon sinks dynamics (Joos et al., 2001). The results for the climate change impact of any substance are given by multiplying the LCI of this substance by its respective GWP, which delivers the results in kg CO₂ equivalent. However, the investigation of the potential climate change impact by the GWP concept may be biased as a strong (high infrared absorption capacity) GHG with short lifetime could have the same results as a weaker GHG with a longer lifetime. In reality, similar emissions of the two gases lead to different temperature change, at a given time (Shine et al., 2005), and so the impact result evaluated by GWP is strongly dependent on the chosen time horizon. Another metric is proposed by Shine and co-workers (2005) which is called Global Temperature Potential (GTP). Their method calculates the relative value of global-mean temperature change of a certain substance with respect to the value of carbon dioxide (in the same conditions). Here also, a time horizon is chosen for the calculation. The results of an LCA study may present an important difference following the choice of the time horizon; this choice is rather a political decision than a scientific one (Shine, 2009).

One of the main limitations in current LCA method is the non-consideration of the time dimension. In the LCIA step, most studies dealing with temporal aspects are dedicated to climate change impact. For example, Cherubini et al. (2011) performed a calculation considering dynamic carbon removal by the biomass, which is a step prior to the calculation of the climate change impact. However, dynamic results for midpoint or endpoint climate change impact are not given as the calculated results are integrated in a single unit-based index. Levasseur et al. (2010) and Kendall (2012) studied time dependency in climate change impact by calculating temporal characterization factors (CF) for substances and applying them to dynamic emissions. Nonetheless, the authors focused on the LCIA

step and modelled simple systems that did not present a complex network of processes (and emissions) as most LCA studies do. The fixed time step and simple input of data for the LCI did not allow the application of a more complex and complete dynamic LCI in their methods. Moreover, the aggregation of the results of GWP leads to a loss of temporal information as the method needs a time horizon to be fixed. Their method is thus definitively dependent on the choice of a time horizon.

The objective of this chapter is to develop a dynamic approach for the calculation of climate change impact within LCA. A brief presentation of the conventional assessment methods and metrics is given as the base for the development of the dynamic approach.

III.2. Method

This section presents the theoretical background of the climate change assessment method in LCA and envisioned by the IPCC (IPCC, 2013), through two indicators: the global warming potential and the global temperature potential.

III.2.1. Modelling of GHG behaviour and effects

To obtain reliable characterisation of gases behaviour and effects in atmosphere, complex deterministic models have been developed to describe the climate system. Climate models consider well-established physical fundamentals and they have been properly reproducing recent and past climate changes features (IPCC, 2007).

Atmosphere-Ocean General Circulation Models (AOGCMs) are generally used to estimate the climate change. AOGCMs describe the climate in a three dimensional grid dividing the globe vertically (atmosphere might be divided in 10 to 20 vertical layers and ocean might be divided in 30) and horizontally with a resolution of 250 to 600 km (IPCC, 2007). There are also simpler models as the “box models” that might be used for fast calculations and evaluations. For instance, box models divide the climate system in boxes (reservoirs) which are linked by flows. The available box models have been validated on the base of AOGCMs and on experimental data.

III.2.1.1. Example of a box model: Bern model for CO₂

IPCC Second assessment Report in 1995 (SAR) adopted the impulse response function from Bern model (Joos et al., 1997) for the calculation of climate change impact metrics. Since then, Bern model is the point of comparison for the several more complex models that have been developed.

The Bern model is a box model where anthropogenic carbon is partitioned between three main reservoirs: atmosphere, ocean and land biosphere (Figure III.1). Atmosphere is considered to be a homogeneous box. The ocean reservoir is described by HILDA model which includes two well-mixed surface boxes, representing low and high-latitude surface water masses, a well-mixed high-latitude deep water box and a diffusive interior reservoir. The terrestrial component includes representation of ground vegetation, wood, detritus and soil (Joos et al., 1997).

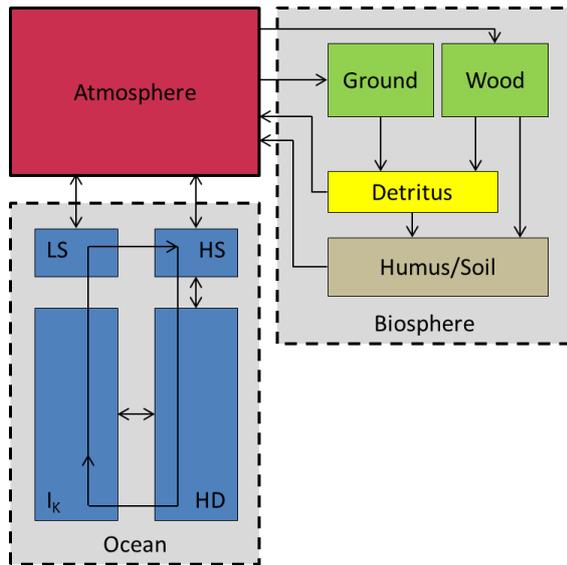


Figure III.1 – Representation of the Bern box-model

III.2.1.2. Impulse response functions

Given the complexity of climate models (AOGCM) and the computational time spent in the calculation, that models cannot be directly used in LCA studies. A simpler way to evaluate the behaviour of substances in environment is the use of box models characterized by specific Impulse Response Functions (IRF).

The idea is to benefit from the dynamic and linear systems mathematics. Considering a complex “black box” system (i.e. there is no available mechanistic representation of the system functioning), the link between the system inputs and outputs can be characterized by an IRF (Figure III.2). IRF is the dynamic output (or system response) for an impulse (or Dirac) input (which can be obtained by experience or simplified modelling). Knowing IRF of a system allows calculating the system’s dynamic response (output $y(t)$) for any variable input $x(t)$, by using the convolution product (Equation III.1):

$$y(t) = \int_{-\infty}^{+\infty} x(t') IRF(t - t') dt' \quad \text{Equation III.1}$$

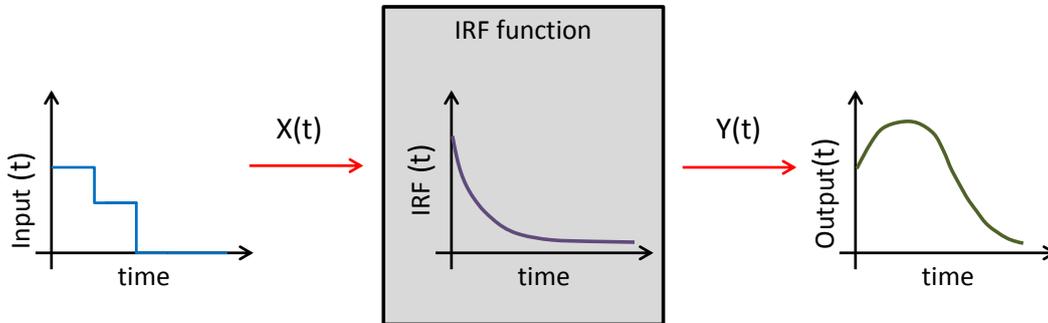


Figure III.2 – Principles of linear dynamic systems representation using IRF

Two main characteristics were represented by the way of dynamic linear systems – IRF functions: 1) the GHG fate, i.e. their distribution in the environmental compartments, and 2) the thermal behaviour of the planet following a thermal flux, leading to a global mean temperature modification.

III.2.1.3. Radiative forcing and global mean temperature change

The distribution of a GHG in the environmental compartments can be represented by a box model like the Bern model in case of CO_2 . Moreover, the dynamic behaviour of boxes (or compartments) can be described by IRF functions specific for each substance. For climate change concerns, it is the atmospheric load (or burden) which must be known. The evolution of the atmospheric burden after the pulse emission of 1 kg of a species s is often written as a sum of decaying exponential functions (Olivié & Peters, 2012):

$$IRF_s(t) = \sum_{n=0}^{n-1} a_n \exp(-t/\tau_n) \quad \text{and} \quad \sum_{n=0} a_n = 1 \quad \text{Equation III.2}$$

Where IRF is the impulse response function characterizing the fate of the substance s , t is time and τ is the substance lifetime.

The radiative forcing is the perturbation of the energy balance of the Earth-atmosphere system (IPCC, 1995) and, for a substance is defined by:

$$RF_s(t) = A_s IRF_s(t) \quad \text{Equation III.3}$$

Where A_s is the specific radiative forcing ($\text{W.m}^{-2}.\text{kg}^{-1}$), IRF_s is the impulse response function for the emission of 1 kg of substance s (defined here above) and RF_s is the radiative forcing (W.m^{-2}) for 1 kg of substance s . We can see that the radiative forcing function has the same shape that the IRF –fate function, A_s being a constant. The radiative forcing is a key parameter for the evaluation of consequences of energy balance perturbation, the global mean surface temperature change for instance.

The simplest model of the global mean surface temperature change, ΔT , for a given global-mean radiative forcing, RF , was presented by Shine and co-workers (2005) (Equation III.4). Their method considers the thermal sensitivity of the climate system and the heat exchange between ocean and atmosphere. Therefore, it also includes the substances concentration decay and the climate system response time scale (IPCC, 2013).

$$C \frac{d\Delta T(t)}{dt} = RF(t) - \frac{\Delta T(t)}{\lambda} \quad \text{Equation III.4}$$

were t representing time, C the heat capacity of the system ($\text{J.K}^{-1}.\text{m}^{-2}$) and λ a climate sensitivity parameter [$\text{K}.\text{W.m}^{-2}$] $^{-1}$, which indicates the change in equilibrium surface temperature per unit radiative forcing change. It is also assumed that λ is a constant that is independent of the particular mechanism causing the radiative forcing. The same authors also presented the general solution of the previous equation:

$$\Delta T(t) = \frac{1}{C} \int_0^t RF(t') \exp\left(\frac{t' - t}{\lambda C}\right) dt' \quad \text{Equation III.5}$$

where d (years) is a time constant that is the result from the multiplication λC . The global-mean surface temperature change for 1kg of substance, ΔT ($\text{K}.\text{kg}^{-1}$), is obtained by analytical resolution for a species s and a time horizon TH :

$$\Delta T(TH) = \frac{A_s}{C(d^{-1} - \tau_s^{-1})} \left[\exp\left(\frac{-TH}{\tau_s}\right) - \exp\left(\frac{-TH}{d}\right) \right] \quad \text{Equation III.6}$$

However, Olivié & Peters (2012) proposed another perspective where the temperature impulse response function, IRF_T , is used. IRF_T is described by a sum of exponential terms:

$$IRF_T(t) = \sum_{n=1}^n \frac{f_n}{d_n} \exp\left(\frac{-t}{d_n}\right) \quad \text{Equation III.7}$$

with the multiplication λC being the sum of time constants d_n (years), and the sum of f_n parameters [$K.(W.m^{-2})^{-1}$] resulting in λ .

IRF_T is independent of the type of GHG, and represents the thermic response of the planet to a unitary impulse of radiative forcing.

III.2.2. Conventional assessment and metrics

Metrics such as Global Warming Potential and Global Temperature Potential were proposed. Their definition is presented below.

III.2.2.1. Global Warming Potential, GWP

Global warming potential is the main metric currently used in LCA that allows the climate change impact calculation. GWP compares the radiative forcing of a gas with those of CO_2 (IPCC, 1990).

The absolute GWP for a specific gas, $AGWP_s$ ($W.m^{-2}.kg^{-1}.year$), is defined by Equation III.8 where TH is the time horizon considered (years).

$$AGWP_s(TH) = \int_0^{TH} RF_s(t) dt \quad \text{Equation III.8}$$

GWP was developed and adopted for use in Kyoto Protocol and is defined by:

$$GWP_s(TH) = \frac{AGWP_s(TH)}{AGWP_{CO_2}(TH)} \quad \text{Equation III.9}$$

The impact calculation in LCA (expresses in $kg CO_2\text{-eq}$) is given in Equation III.10 where the climate change impact is the sum of the products between the inventory mass (G_s) and the GWP_s of all substances s concerned, and for a given time horizon TH:

$$Climate\ Change(TH) = \sum_s GWP_s(TH) G_s \quad \text{Equation III.10}$$

III.2.2.2. Global Temperature Potential, GTP

Shine et al., (2005) proposed another metric called Global Temperature Potential that compares the global-mean temperature change due to a gas emission, at a certain time after the emission, with the global-mean temperature change for CO₂

According to Olivie & Peters (2012), the expression of Absolute Global Temperature Potential can be represented as follows:

$$AGTP_s(TH) = \int_0^{TH} RF_s(t) IRF_T(TH - t) dt \quad \text{Equation III.11}$$

The GTP, which is the normalization of the absolute global temperature potential of a gas *s* by a reference gas (CO₂ by convention), is represented by:

$$GTP_s(TH) = \frac{AGTP_s(TH)}{AGTP_{CO_2}(TH)} \quad \text{Equation III.12}$$

The climate change impact (expresses in kg CO₂-eq) based in GTP can be defined by:

$$Climate\ Change(TH) = \sum_s GTP_s(TH) G_s \quad \text{Equation III.13}$$

The parameters for the calculation of GWP and GTP can be found in SI II.1, 2 and 3.

In determining the characterization factors in conventional LCIA, both metrics are based on the following constraints: 1) the gas emission follows a unit impulse at time zero, and 2) a time horizon is fixed. Thus, the characterization factors (GWP, GTP) are numbers determined for very particular conditions. Moreover, when the impact result is calculated, the gas emission dynamics (*g(t)*) is not considered.

III.2.3. Time consideration in climate change impact

The environmental interventions usually present complex temporal behaviour that requires a rigorous resolution approach. As described in section (LCI), the dynamic inventory data can be defined as a time dependent function in an analytical manner or as numerical values at given time values.

In this section, two indicators are proposed for the impact category climate change, in a dynamic approach: 1) the dynamic radiative forcing (instantaneous or current, and cumulated), and 2) the global mean temperature change.

III.2.3.1. Dynamic behaviour of GHG

In case of a dynamic approach, it is necessary to consider the time variation of the environmental burdens. The atmospheric burden B_s (kg), in response to any emission scenario g_s (kg), can be written as a convolution product using the IRF for the substance fate in environment:

$$B_s(t) = \int_{t_0}^t g_s(t') IRF_s(t - t') dt' \quad \text{Equation III.14}$$

where t_0 represents the initial time of emission, t is a given point on the time scale and t' is the time variable for convolution.

General IRF function was given in Equation III.2. However particular functions also exist for some substances. Moreover, chemical transformations shall also be considered, as in the case of methane.

III.2.3.2. Consideration of methane oxidation

After the release of methane in atmosphere, one of the reactions that methane undergoes is an oxidation. Hydroxyl (OH) is the main compound responsible for the oxidation of methane. The final products are carbon dioxide and methanol, formaldehyde and carbon monoxide as intermediate products. However, not every molecule of methane is converted in CO_2 as the intermediate products may be deposited at the soil surface or disintegrated (Boucher et al., 2009).

In order to take it into account, as proposed by Ericsson et al. (2013), the carbon dioxide produced by methane conversion in the oxidation reaction should be accounted in the dynamic inventory. The amount of CO_2 ($g_{CH_4TOCO_2}$) which is produced from the oxidation of methane in the time interval δt is given by:

$$g_{CH_4 to CO_2}(t) = (B_{CH_4}(t) - B_{CH_4}(t - \delta t)) * \frac{MM_{CO_2}}{MM_{CH_4}} \quad \text{Equation III.15}$$

Where MM is the molar weight and B_{CH_4} is the atmospheric burden of methane. Finally, the updated value of CO_2 in the inventory is:

$$g_{CO_2 updated}(t) = g_{CO_2}(t) + g_{CH_4 to CO_2}(t) \quad \text{Equation III.16}$$

Boucher et al. (2009) stated that the quantity of methane which converts to CO_2 is uncertain. In their study, they considered the amount transformed between 50 and 100 percent. In this study, all methane is considered to be converted to carbon dioxide.

III.2.3.3. *Dynamic alternative to Global Warming Potential*

The radiative forcing, RF_s , of a gas s is the product of its radiative efficiency, A_s , and the perturbation in its abundance (or its burden) Joos et al. (2013). In this general formula, RF is calculated in function of any emission $g(t)$ and of the intrinsic system's behaviour described by its IRF.

$$RF_s(t) = A_s(t)B_s(t) = A_s(t) \int_{t_0}^t g_s(t')IRF_s(t - t')dt' \quad \text{Equation III.17}$$

For sufficiently small emission and approximately constant background conditions the radiative efficiency, A_s , can be approximated as time-invariant (Joos et al., 2013). The integral can be discretized as follows:

$$RF_s(t) = \sum_{t'=t_0}^t A_s g_s(t') IRF_s(t - t') \Delta t \quad \text{Equation III.18}$$

$RF(t)$ represents the current (at the moment t) dynamic radiative forcing.

The dynamic radiative forcing for all the substances concerned is given by:

$$n_{radiative forcing}(t) = \sum_s RF_s(t) \quad \text{Equation III.19}$$

The cumulated radiative forcing $n_{\text{radiative forcing, cumul}}(T)$, calculated at a span time T , is given by:

$$n_{\text{radiative forcing, cumul}}(T) = \sum_{t=0}^T n_{\text{radiative forcing}}(t) \quad \text{Equation III.20}$$

III.2.3.4. *Dynamic alternative to Global Temperature Potential*

The second indicator can be modelled in the dynamic approach by using a real radiative forcing RF instead of the particular RF due to an impulse emission. In general formula below, the new impact indicator $n_{\text{temperature, s}}(t)$ is calculated for any dynamic emission $g(t)$ of substance s :

$$n_{\text{temperature, s}}(t) = \int_{t_0}^t \left(\int_{t_0}^{t'} A_s g_s(t') \text{IRF}_s(t - t') dt' \right) \text{IRF}_T(t - t') dt' \quad \text{Equation III.21}$$

$n_{\text{temperature, s}}(t)$ is the global mean temperature change ΔT (in K) calculated at a given moment t , for a substance s , IRF_T is the temperature impulse response function of the planet in $\text{K} (\text{W} \cdot \text{m}^2)^{-1}$.

Aggregated values for all substances emitted can be calculated by:

$$n_{\text{temperature}}(t) = \sum_s n_{\text{temperature, s}}(t) \quad \text{Equation III.22}$$

Where $n_{\text{temperature}}(t)$ is the mean temperature change at time t due to all concerned substances. It is noticeable that the indicator calculation does not depend on a time frame or time horizon, but, instead, the value of the indicator is obtained at any desired time value T , $n_{\text{temperature}}(T)$.

The dynamic mean temperature change approach is more suitable for a dynamic LCA study as it gives an end-point metric with values calculated for any point in time T . Also, the interpretation of this indicator is easier as the unit and dimension of the mean temperature change is more simple and popular than the ones of radiative forcing.

III.3. Results and discussion

Carbon dioxide and methane were considered as testbed cases. For each substance, two emission profiles were considered: A) an emission over 20 years in “air, undefined” compartment. It was described by a simple step behaviour (Figure III.3 curve A): 0.04 kg.year⁻¹ constant flow during the first 10 years, then a constant flow of 0.06 kg.year⁻¹ between year 10 and 20, zero after year 20; B) a constant emission (Figure III.3 curve B) with a constant flow of 0.01 kg.year⁻¹ over 100 years in “air, undefined” compartment. For both cases the total mass of emission is 1 kg (time integral of the emission flow).

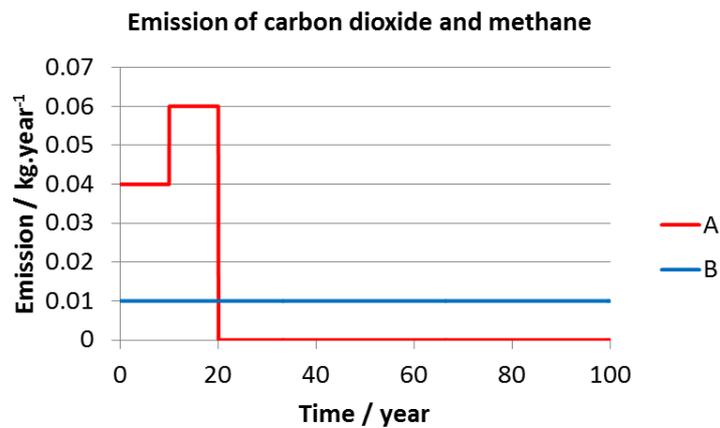


Figure III.3 – Step emission profile (A) and continuous emission profile (B) for carbon dioxide and methane.

Figure III.4 shows the results of global mean temperature change (Equation III.21) for cases A and B, for both carbon dioxide and methane, over a time span of 100 years.

Considering the case A for carbon dioxide (Figure III.4.I.A), the mean temperature change reaches a value of 5.56E-16 K at year 100. This value corresponds to 82% of the maximum value (6.77E-16 K). For case B (Figure III.4.I.B), the dynamic temperature change increases almost linearly reaching a value of 5.88E-16 K at the time span considered. The difference in the result is not significant at year 100; however, the impact is notably higher for case A in the first decades. It is easy to observe that the maximum ΔT will be obtained in case B at longer time span, depending on the emission duration (curve B, Figure III.4).

For the case A of methane emission (Figure III.4.II.A), the mean temperature decreases and reach a value of 2.61E-15 K at the time span of 100 years, which is not significant comparing to the maximum value 5.30E-14 K. In this case, a peak of temperature change could be seen around year 25 (five years

after the last methane release). The delay observed between the last emission and the maximum temperature is due to the thermic behaviour of the planet, represented by the temperature impulse function. For the case B (Figure III.4.II.B), the mean temperature change increased until the time span and reached a value of $1.85E-14$ K. As the emissions were distributed evenly during 100 years, the effect of the temperature impulse function was also distributed which lead to a continuous increase. The values at 100 years are significantly different from case B having the highest impact; however, until year 50 the mean temperature change was even three times higher for case A than for case B.

It was thus demonstrated that a maximum value can be reached before the end of the time span (time horizon in conventional LCA) and few years after the end of the emissions, which shows that the conventional method may hide important information for the impact analysis: when the maximum happens and its amplitude.

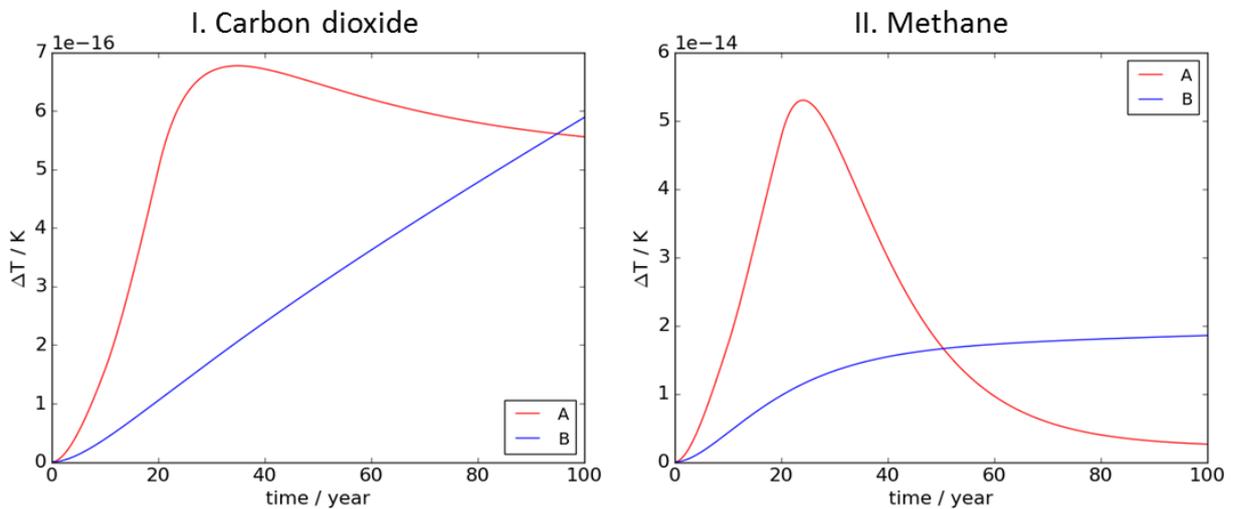


Figure III.4 – Dynamic mean temperature change calculated over 100 years for carbon dioxide emission (I) and methane emission (II) for a step profile emission over 20 years (A) and a continuous profile emission over 100 years (B).

Figure III.5 shows the results of dynamic cumulated radiative forcing (Equation III.19) for cases A and B for both carbon dioxide and methane over a span time of 100 years.

Considering the case A for carbon dioxide (Figure III.5.I), the cumulated radiative forcing reaches a value of $8.36E-14$ $Wm^{-2}day$ by year 100. For case B, the cumulated radiative forcing reaches a value of $5.09E-14$ $Wm^{-2}day$ at the same time. The difference will remain stable from the time span to the following years due to the airborne fraction of CO_2 .

For the case A of methane emission (Figure III.5.II), the cumulated radiative forcing reaches a value of $2.60E-12$ $Wm^{-2}day$ at 100 years. As the last methane release takes place at year 20 and its lifetime is

short, the cumulated radiative forcing results for the last years remain constant. For the case B, the cumulated radiative forcing reaches a value of $2.28\text{E-}12 \text{ Wm}^{-2}\text{.day}$. The difference between the cumulated radiative forcing of the two emission profiles decreases when reaching 100 years and inverses the tendency due to the tardive emission of methane. If a very longer time span were chosen, the results would reach similar values, determined by the residual CO_2 coming from the methane oxidation.

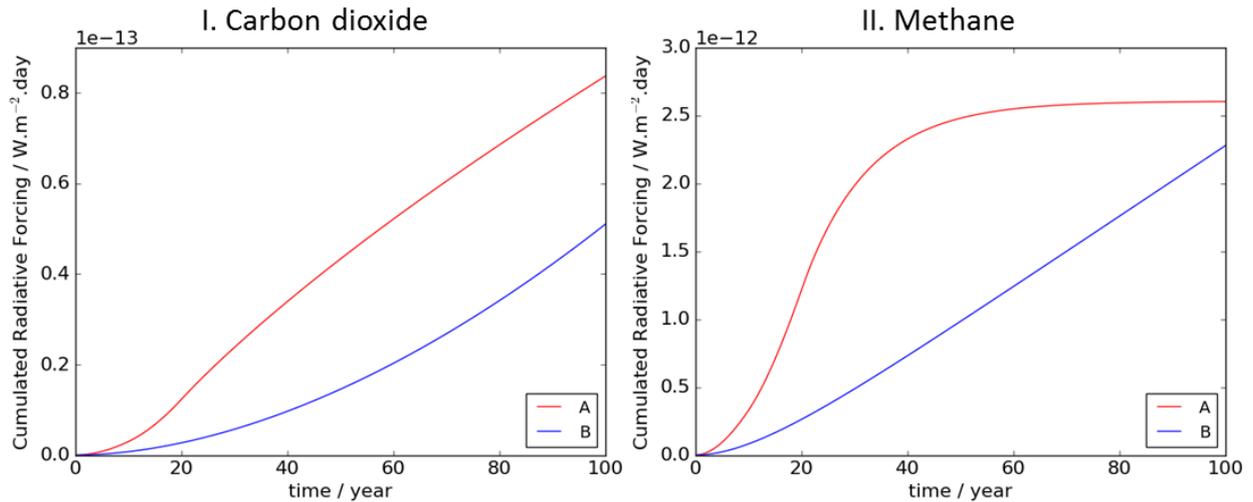


Figure III.5 – Dynamic cumulated radiative forcing calculated over 100 years for carbon dioxide emission (I) and methane emission (II) for a step profile emission over 20 years (A) and a continuous profile emission over 100 years (B).

In conclusion, both dynamic climate change indicators showed that the dynamic results for two different emission profiles with the same conventional inventory results can be very different. Considering only the results at the time span chosen (horizon time for conventional studies), radiative forcing and temperature change methods presented opposite results: while for temperature change the case B presented the highest impacts at year 100, for radiative forcing it was the case A. At the contrary, for another point in time chosen before 100 years, both indicators give the same ranking. It is noticeable that considering the results only at a fixed time horizon can lead to misinterpretation of the impact deployment; investigating the impact results over all the time frame and moving the time span limits is important in order to capture all the specificities of the studied system.

Table III.1 shows the conventional and dynamic mean temperature change and radiative forcing results for a time frame of 100 years. In the case of mean temperature change for carbon dioxide, the values found through the dynamic evaluation are quite similar to those obtained from the conventional method. The results at year 100 might undergo mostly the influence of the airborne fraction of CO_2 which is still the same for dynamic and conventional methods when the emission duration is small

with respect to the total time span. In the case of methane, the dynamic results for 100 year span time are higher than the conventional results. This can be explained by the fact that the last emissions took place late in time comparing to the consideration of an impulse emission at time zero in the conventional method (last emission at year 20 for case A and 100 for case B).

In the case of cumulated radiative forcing for carbon dioxide, the dynamic results were smaller than the conventional results. The conventional method consideration of the CO₂ emission taking place at year 0 overestimates the results as it accounts impacts which would happen after the time horizon if a dynamic distribution of emissions was considered. In the case of methane, the dynamic results for the case A, calculated over 100 years, are similar to the conventional results. However, the dynamic results for the case B were smaller which is explained by the fact that the last emissions of methane were not entirely accounted in the impact as this substance stays in atmosphere for several years after the end of emissions.

Table III.1– Dynamic mean temperature change and cumulated radiative forcing results for the emission of carbon dioxide and methane.

Emission		Mean temperature change		Radiative forcing	
		Conventional 100 years	Dynamic 100 years	Conventional 100 years	Dynamic 100 years
Carbon dioxide	A		5.6E-16		8.36E-14
	B	5.5E-16	5.88e-16	9.17E-14	5.09E-14
Methane	A		2.61E-15		2.60E-12
	B	2.34E-15	1.85E-14	2.61E-12	2.28E-12

Levasseur et al. (2014) also proposed a dynamic climate change impact which is based on the metric Global Warming Potential. After studying the behaviour of carbon dioxide, the authors concluded that the results of conventional climate change impact are significantly different from the values resulting from a dynamic study: emissions can be delayed in comparison to a conventional method in which the emissions are considered as pulse at time zero. However, in their method, the results of dynamic global warming impact are aggregated at the end which leads to a loss of important temporal information. At the contrary, the model developed here proposes two dynamically calculated indicators, allows the modification of the time step size for the calculation and is not based in pre-calculated characterization factor. The calculation can be performed for the desired time frame and didn't use a reference substance.

III.4. Method conclusion

The climate change dynamic impact proposed by this study, obtained by the adaptation of the radiative forcing and mean temperature change parameters, gives midpoint and endpoint results which can be analysed for every point in time. Both indicators are physical characteristics involved in the cause to effect chain of the climate process.

The indicator based on the radiative forcing considers the GHG dynamics in the environmental compartments. The indicator based on the global mean temperature change adds to the previous the dynamics of thermic phenomena on the planet.

The approach of box models was used. Dynamic indicators were modelled as the outputs of the box-model, using the impulse response function method and the convolution product between inputs and IRF.

Important features were highlighted in this approach: 1) a maximum value of temperature change is reached at some point depending on the emission profile, which is neglected in the conventional method; 2) the comparison with the conventional method results shown that a fixed horizon time is arbitrary with respect to the studied system and leads to different rankings between scenarios when the time horizon is changed; 3) the proposed method is not based in pre-calculated characterization factor, the calculation can be performed for the desired time frame and did not use a reference substance.

Case study: Environmental assessment of bioenergy production from microalgae based systems

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Abstract

Microalgae have been studied as a potential alternative raw material in bioenergy production and various technologies have been proposed to transform the algal biomass into energy products. In this study, two bioenergy production systems were modelled to assess the environmental efficiency of energy production from microalgae: a biodiesel system and a biogas system. Cumulative energy demand, life cycle assessment and dynamic life cycle assessment for climate change evaluation were used to evaluate the environmental footprint of the production systems. Conventional systems for electricity, heat and diesel production were considered for comparison.

The energy balance showed that the supercritical extraction and drying steps were the most energy consuming unit operations in biodiesel production and further developments of technologies might be envisaged. Life cycle assessment showed that climate change was the main contributor to impacts on human health and ecosystem quality. Also, heat from biogas was the only product that proved to have a satisfactory environmental potential with regard to other conventional production systems. Finally, dynamic climate change evaluation revealed no carbon sequestration in the microalgae system.

Keywords: Life Cycle Assessment, Bioenergy, Microalgae, Dynamic climate change model, Renewable resource

III.5. Introduction

Energy production is the main contributor to climate change, accounting for 47% of global greenhouse gas (GHG) emissions in 2010. In addition, the transportation sector is responsible for approximately 14% of the global warming effect as almost all the energy consumed (approximately 95%) in transport systems comes from fossil fuels (IPCC, 2013). To reduce the impact of the use of fossil energy, bioenergy policies have been implemented in Europe. The Renewable Energy Directive (RED) establishes national energy targets for countries in the European Union (EU). In France, a target of 23% of renewable energies in the total energy consumption is envisaged for 2020. The estimated bioenergy consumption in France in 2015 is 1.35×10^5 TJ in biofuels and 6.3×10^5 TJ for heating and cooling. By 2020, an increase of about 26.3% is expected for biofuels and 31.1% for heating and cooling (RED, 2009).

The feedstock for first and second generation biofuels comes mostly from edible crops. This scenario has raised important questions concerning the competition between food and biofuel production for arable land and also the fact that fuels from crops can lead to a higher global warming effect than the use of fossil fuel (Collet et al., 2011). In this context, microalgae have been pointed out as an interesting source of energy that does not enter into significant competition with food. Fuels derived from microalgae, which present advantages such as a very rapid growth compared to other oil crops, high photosynthetic yields and high ability to cumulate lipids, are being considered as third generation fuels (Chisti, 2007). The photosynthetic yield for microalgae is about 3-8% of solar energy transformed to biomass whereas, for terrestrial plants, it is about 0.5% (Huntley and Redalje, 2007; Li et al., 2008). Moreover, some studies (Francisco et al., 2010; Poloo-Aikins et al., 2010) have also claimed that bioenergy production from microalgae results in carbon sequestration (defined as the capture and long-term storage of atmospheric carbon dioxide).

A variety of technologies for biodiesel production have been investigated and others are under study. The key steps of biodiesel production from microalgae are the production of the microorganisms, lipid extraction and transesterification. Conventional lipid extraction usually involves hexane, which is flammable and toxic and is believed to have adverse health and environmental effects (Cheng et al., 2011). Conventional transesterification includes the use of catalysts, which has at least two drawbacks: it is a relatively time consuming process and the product has to be purified to remove catalyst and saponified compounds (Saka and Kusdiana, 2001). Environmental assessments of biodiesel manufacture from microalgae using such processes are available in the literature (Lardon et al., 2009; Sander and Murthy, 2010).

Supercritical fluid processes, such as extraction (Cheng et al., 2011; Mendes et al., 1995; Nikitine et al., 2009) and transesterification (Saka and Kusdiana, 2001; Bunyakiat et al., 2006; Dermibas, 2005), have been studied as possible alternatives to the conventional methods as they avoid the weaknesses mentioned above.

Furthermore, microalgae can also be an interesting source of biogas. This process, relatively simple compared to biodiesel production, does not require concentration and oil extraction steps and could thus avoid significant energy consumption (Collet et al., 2011).

In this context, the present study aims to evaluate the environmental efficiency of two systems for obtaining bioenergy from microalgae, using different and complementary environmental assessment tools and methods. The bioenergy systems chosen are of very different technological complexities: 1) biodiesel (BD) using supercritical extraction/transesterification and 2) biogas (BG) for cogeneration.

The following assessment methods were applied: i) Energy balance analysis of the production process at the process level (EB) and over the process life cycle using a Cumulated Energy Demand (CED) indicator, ii) Life Cycle Assessment (LCA) to evaluate the environmental impacts of the bioenergy over its life cycle (i.e. direct and indirect impacts generated by the bioenergy production and utilization, involving all natural resources consumed and all harmful substances emitted), and iii) Dynamic Life Cycle Assessment (DLCA) to demonstrate the possible existence of carbon sequestration by microalgae.

III.6. Methodology

III.6.1. Bioenergy production systems

The bioenergy production systems investigated in this study are: i) the biodiesel process (BD), in which electricity and heat are also produced as well as biodiesel, and ii) the biogas process (BG), in which heat and electricity are produced (Figure III.6).

The microalgae culture and harvesting steps were considered to be similar for both systems (Figure III.7). In BD, the harvested biomass is dried and sent to the lipid extraction step, which uses supercritical carbon dioxide as the solvent. The extracted oil is used in supercritical transesterification with methanol as a reactant and, finally, the biodiesel obtained is purified by distillation. The biomass remaining after extraction is sent to anaerobic digestion, in which biogas is produced and transformed into electricity and heat by cogeneration. In BG, the algal biomass is directly used in an anaerobic digester for biogas production and subsequently for electricity and heat production by cogeneration. Details of the processes are presented below.

To the best of our knowledge, no full scale plants exist for biodiesel production from microalgae. In order to apply the aforementioned assessment methods, a mass and energy balance was calculated on the basis of unit process modelling and available literature data.

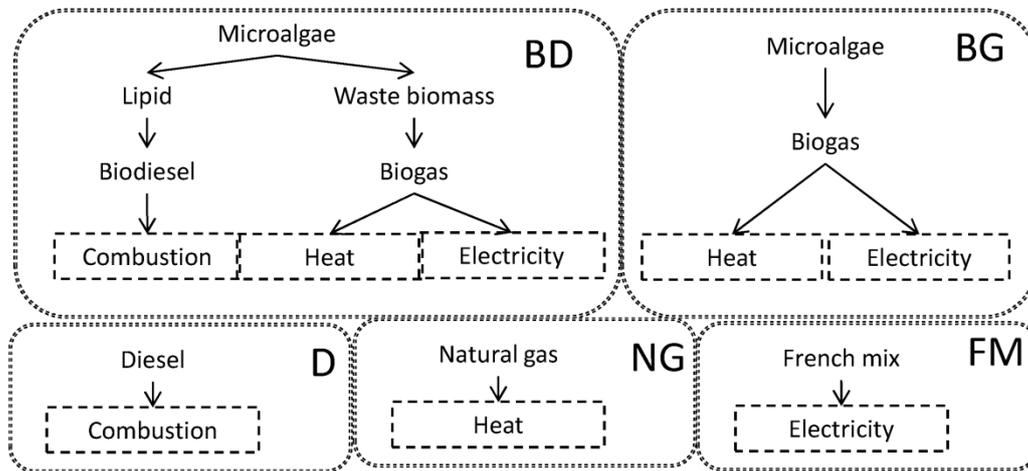


Figure III.6 – Production systems considered in this study

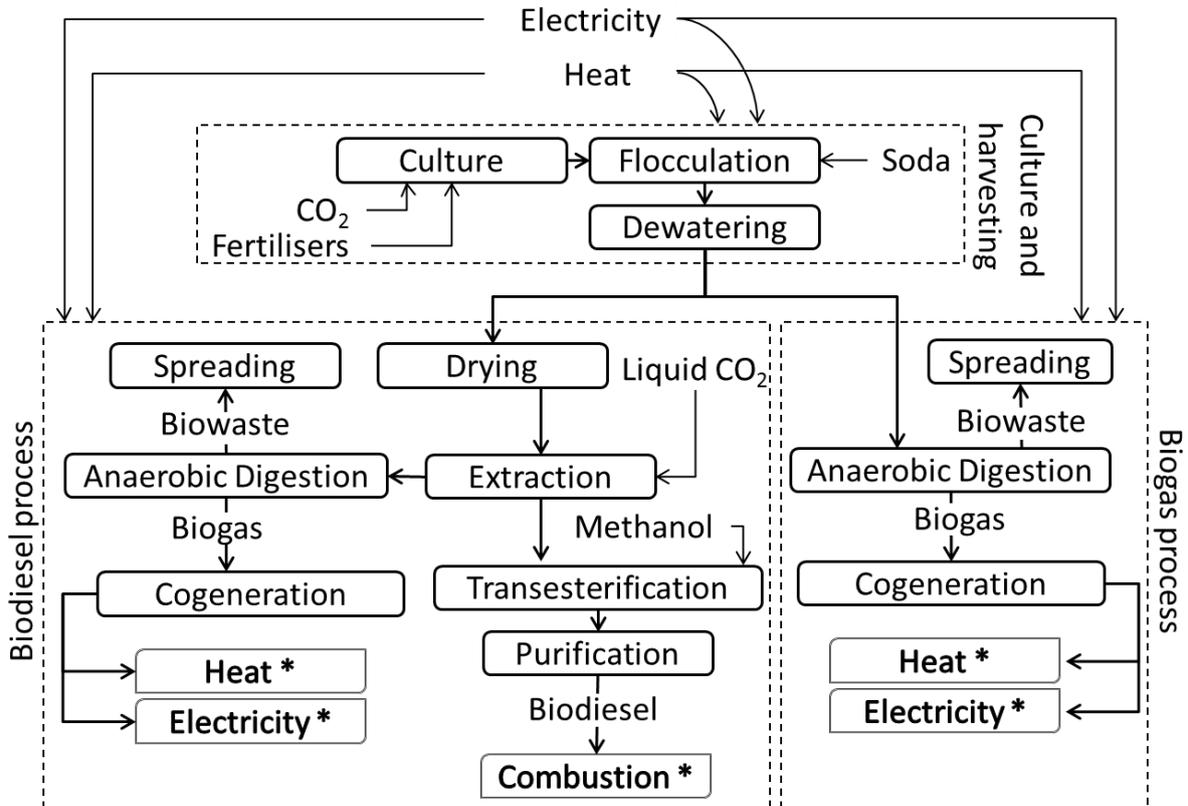


Figure III.7 – Biodiesel and biogas modelled processes (*) represents final product

III.6.2. Energy balance and analysis

As pointed out above, the energy balances of BG and BD were calculated for an industrial scale, and the Energy Return On Investment (EROI) (Equation III.23) indicator was used to evaluate the performance of each energy production system.

$$EOIR = \frac{\text{Energy produced}}{\text{Energy invested}} \quad \text{Equation III.23}$$

The Cumulated Energy Demand (CED) indicator (Jungbluth et al., 2007) was calculated using the Life Cycle Inventory (see III.2.3) in order to show the contribution of natural energy resources to global energy consumption over the whole life cycle of the process.

III.6.3. Life Cycle Assessment

The Life Cycle Assessment (LCA) method is defined by ISO 14040 as the "compilation and evaluation of the inputs, outputs and potential environmental impacts of a product system throughout its life cycle" (ISO 14040, 2006a). LCA is applied following four steps (ISO 14040, 2006a, 2006b): the definition of goal & scope, the building of a Life Cycle Inventory (LCI), the Life Cycle Impact Assessment (LCIA), and the interpretation of the results.

Goal and scope. From an LCA point of view, our objective was to evaluate the potential environmental impacts of three kinds of energy obtained from microalgae: energy in biodiesel, electricity, and heat. These energy types are obtained in BD and BG production systems.

Then, based on the product functions, comparisons will be made with conventional production of diesel energy (D), French mix electricity (FM), and heat from natural gas (NG). The functional unit is 1 MJ. It should be noted here that BD and BG systems cannot be compared directly as they supply different types and proportions of energy products.

Since both modelled process lead to the production of several co-products, a mass allocation was performed in the extraction step in order to share the environmental burdens among the different co-products. For electricity and heat production, the default allocation (exergy) for the unit process of cogeneration in the Ecoinvent v2.2database (Frischknecht et al., 2005) was used.

Systems boundaries for the chosen functions were as large as possible (cradle to grave), including the functioning of the processes (foreground and background) and the infrastructure when data were available. The foreground processes are those for which case-specific data are used (i.e. BG and BD)

while the background processes are processes of the life cycle for which generic (or more general) information is used.

Life Cycle Inventory. The mass and energy balances and inventories were obtained for BG and BD by process modelling considering the operating conditions and productivity described in 2.5 and SI (section SI III.1 to SI III.6). When necessary, complementary information was obtained from the literature.

Inventories for background processes (production of chemicals, electricity, transport, infrastructure) were taken from the Ecoinvent v2.2 database (Frischknecht et al., 2005).

Life Cycle Impact Assessment. The impact evaluation method used was ReCiPe 2008 (Goedkoop et al., 2009). This method translates the LCI into impact results at midpoint (evaluates environmental problems) and at endpoint as damage to three areas of protection: natural resources, human health and ecosystem quality. LCA was performed with the Umberto[®] 5.6 software.

III.6.4. Dynamic LCA - climate change

Climate change impact is currently evaluated in LCA and related methods (e.g. Carbon Footprint), by the Global Warming Potential (GWP), based on radiative forcing. Shine et al. (2005) propose a metric called Global Temperature Change (GTP), based on the variation of the global mean surface temperature due to greenhouse gas (GHG) emission. These parameters are calculated at arbitrary time horizons (commonly at 100 years) without real consideration of the evolution of the gas emissions from the studied system over time and of the gas dynamics in the environmental compartments.

In this work, a model was applied to evaluate the GTP varying according to time, considering the emission dynamics over the life cycle of the system studied and the dynamic behaviour of the three main GHG, i.e. CO₂, N₂O and CH₄.

The dynamic LCI was modelled following the method proposed by Tiruta-Barna et al. (2016), considering the temporal behaviour of the foreground processes (BD and BG) and the temporal behaviour of the supply chain (i.e. the background processes constituting the life cycle of BD and BG). Concerning GHG dynamic behaviour, the models described by Joos et al. (2013) and IPCC (2013) were used.

III.6.5. Process description

In this section, the processes involved in BG and BD production systems, and represented in the global flowsheet of Figure III.7, are described along with the necessary information for LCI building.

Cultivation and harvesting

The microalgae strain chosen to be used as raw material was *Dunaliella salina*, which is known for its ability to produce β -carotene but is also able to accumulate lipids and thus to provide an alternative for the production of biodiesel (Mishra et al., 2008). This strain also has advantages such as resistance to open conditions and the use of sea water for growth, thus decreasing the consumption of fresh water (Li et al., 2008).

Culture of *Dunaliella salina* was modelled as taking place in open ponds with a total surface of 100 ha (10^6 m²). The location of the culture process was in the south of France, at the seaside, with large amounts of sunlight, and near a thermal power plant which could provide CO₂ for the culture. The flue gas from thermal power plant (13.6% CO₂ by mass as in Brown, 1996) was injected into the race wheel ponds, where the water was impelled by paddlewheels.

The production rate for *Dunaliella salina* was considered to be 0.03 kg m⁻²d⁻¹ and the number of microalgae doubled every 12 h (Borowitzka, 1990). This led to a production of 3×10^4 kg biomass day⁻¹ and a biomass concentration of 0.4 kg m⁻³. According to Renaud et al. (1994), the lipid content of this microalgae strain is about 28.1% of dry biomass. For the nutriment requirement, a general assumption of the microalgae formula (CH_{1.83}O_{0.48}N_{0.11}P_{0.01}) as found in Grobbelaar (2004 as cited in Chisti, 2007) was considered. Industrial fertilizers were used to provide stable conditions for microalgae to grow, Ammonium nitrate was chosen as a source of nitrogen and single superphosphate as a source of phosphorus. Values for the distance over which the fertilizers were transported from regional storage to the main process site for France were considered to be similar to the distances found in Nemeck and Haji (2007) for Switzerland. Race wheel ponds were designed to be 100 m long, 10 m wide and 0.30 m deep and were constructed in concrete covered by a PVC liner (Collet et al., 2011; Lardon et al., 2009). Energy consumption of the cultivation step was 0.817 MJ of electricity per kg of dry microalgae (Kadam, 2001).

A flocculation step was necessary to collect the microalgae. A process based on the works of Besson and Guiraud (2013) was selected, where the flotation of algae was induced by adjusting the pH through an addition sodium hydroxide (0.9 kg NaOH per kg of dry biomass). This process ensured a recovery efficiency of 90% and a concentration factor of 20, allowing biomass to be collected with approximately 1% of dry matter. Then the water content was reduced in a volute dewatering press to reach 20% of dry matter.

At this stage, the biomass could be used to produce biogas in the BG process.

In case of BD, the microalgae were dried on a belt dryer. According to Lardon et al. (2009), the belt dryer is one of the least energy demanding processes (compared with other systems, e.g. sludge drying in a wastewater treatment plant).

Extraction and Transesterification

Supercritical CO₂ extraction was chosen because of its effectiveness in comparison with other extraction techniques (Li et al., 2014). The process takes place at a pressure ranging from 15 to 40 MPa and a temperature between 313 and 333 K (Cheng et al., 2011; Mendes et al., 1995; Nikitine et al., 2009), which consumes energy. Energy consumption was calculated as 12.6 MJ electricity and 46 MJ heat for the extraction of 1 kg of oil (see SI III). CO₂ is recycled in the process; however a certain quantity must be added periodically to upgrade the solvent quality.

Transesterification by supercritical alcohol presents several advantages over other methods, such as fast reaction rates and a catalyst-free reaction. The reaction conditions are: 623 K and 19 MPa with a methanol flow of 1.668 kg per kg of biodiesel produced (Saka and Kusdiana, 2001). The energy required for the production of 1 kg of biodiesel was calculated at 0.032 MJ electricity and 2.4 MJ heat (see SI III).

Distillation is used to remove impurities in biodiesel and to reach a commercial degree of purity. The energy consumption for the distillation of biodiesel is estimated at 1.24 MJ heat per kg of biodiesel (Glisic and Skala, 2009).

Digestion and Cogeneration

Digestion of biomass for biogas production followed by energy recovery by cogeneration is considered in both BD and BG production systems.

In the case of BD, biomass waste from extraction can be used with glycerol to produce biogas. The use of glycerol is a possibility that can increase the methane yield in the digestion by 4% to 7% (Ehimen et al., 2009).

Collet et al. (2011) have argued that, with a retention time longer than 46 days, a methanisation yield higher than 75% of the maximal biological potential can be reached. The maximum methanisation yield was estimated in this work using the molecular formula of the microalgae and the method described by Sialve et al. (2009) (see SI III). Based on Collet et al. (2011), the energy required for the production of 1 kg of CH₄ was estimated at 2.642 MJ electricity and 13.482 MJ heat.

Biogas has been used in a cogeneration unit with a production capacity of 160 kW of electricity where 0.32 MJ of electricity and 0.55 MJ of heat were produced per MJ of biogas burned (Frischknecht et al., 2005). The remaining biomass could be used as an agricultural fertilizer thanks to its nitrogen and phosphorus content. The most suitable system to spread the material remaining after digestion was a vacuum tanker. Direct pollutant emissions due to spreading were considered to be similar to those for spreading sludge from a wastewater treatment plant (Doka, 2009).

In the case of BG, the dewatered algal biomass is sent to anaerobic digestion. The energy required per kg of CH₄ produced is estimated at 2.642 MJ electricity and 13.482 MJ heat, on the basis of Collet et al.'s (2011) work. Then, the biogas obtained is directed to a cogeneration unit where 0.32 MJ of electricity and 0.55 MJ of heat are produced per MJ of biogas burned. The remaining biomass can be spread on agricultural land to take advantage of its nitrogen and phosphorus content.

For the LCI, heat is considered to be produced from natural gas and all electricity consumed is considered to be produced in France (conventional French mix).

Temporal characteristics

Concerning the foreground process system, the time for the growth of microalgae in the culture step was taken to be 4 days as suggested by Borowitzka & Borowitzka (1988 as cited in Sander and Murthy, 2010). Retention time in the digestion step was considered to be 46 days (Collet et al., 2011). Other unit processes were assumed to take 1 day each. The delay between unit processes was assumed to be zero as the time between unit processes was negligible. The lifetimes of factories for foreground processes were set at 10 years, and the construction of infrastructures and plant took place one year before the start of the operation. The pollutant emissions from different processes were considered constant over the time that the process was running. The temporal characteristics of processes involved in the life cycle of BD and BG were those defined in the DLCA method proposed by Tiruta-Barna et al. (2016) (see SI III).

III.7. Results and discussion

III.7.1. Energy balance and analysis

The net energy value is negative for BD (Table III.2). The most important contributor to energy consumption is the supercritical extraction. The large amount of CO₂ used as the solvent increased the energy demand. Also, a large quantity of energy was required to reach the critical parameters (pressure of 40 MPa). Even though this process is widely used in industry, e.g. in the manufacture of food and pharmaceuticals, it was not suitable for bioenergy production. The other important contributor to

energy consumption was the biomass drying step. Those two processes accounted for 70% of all energy consumption in the BD process. On the other hand, supercritical transesterification presented low energy consumption, and contributed only 2% to the total energy demand.

Table III.2 – Energy balance for the production of 1GJ of biodiesel in the BD process. (For the BG process, the same production of biomass was assumed as in the BD process.)

Process	Energy	BD	BG
Consumption (MJ)			
Culture	Electricity	98.4	98.4
Flocculation	Electricity	157	157
Dewatering	Electricity	26	26
Drying	Electricity	520	-
Supercritical Extraction	Electricity	453	-
	Heat	769	-
Supercritical transesterification	Electricity	0.85	-
	Heat	63.5	-
Purification	Heat	32.9	-
Digestion	Electricity	31.4	42
	Heat	197.9	265.3
Production (MJ)			
Combustion	-	1000	
Cogeneration	Heat	261	573
	Electricity	448	985
Total (MJ)			
Consumption	-	2350	588.7
Production	-	1709	1558
Net (MJ)	-	-644	969.3
EROI		0.727	2.647

Only BG showed potential as an alternative source of energy. The net production of energy in the biogas process was positive. The EROI indicator was higher than 1 only for the BG system. EROI confirmed the non-efficiency of BD as an energy production system.

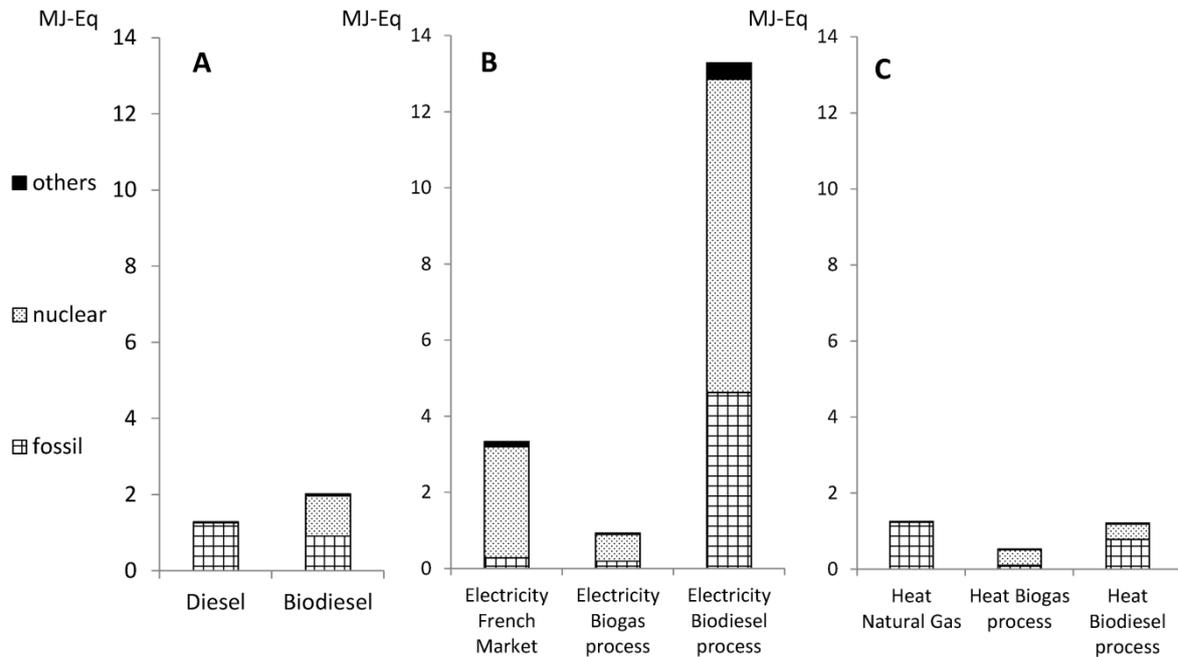


Figure III.8 – Cumulative Energy Demand for: (A) Fuel energy production, (B) Electricity production, and (C) Heat production

Figure III.8 presents the CED results for the production of 1 MJ of each product (biodiesel, electricity and heat). CED takes all energy resources (fossil, nuclear, and renewable: sun, wind, hydropower, wood, etc.) used over the life cycle of the product into account. Thus, it considers not only the energy balance of the studied production system but also the indirect energy consumption in the background processes that form part of the life cycle. For this indicator, the bioenergy from BD and BG was compared to the conventional energy of the same type (products having the same function, following the LCA perspective), i.e. diesel, French mix electricity, and heat from natural gas.

Figure III.8.A shows that the BD life cycle consumes almost twice as much energy as the life cycle of conventional diesel. For heat production (Figure III.8.C), while natural gas and BD consume almost the same amount of energy, BG consumes significantly less for the whole life cycle. For electricity production (Figure III.8.B), BG consumes significantly less energy than the other two processes. CED confirmed the large quantity of energy used in the BD system, especially in the expensive lipid extraction step.

The French electricity grid was chosen as the source of electricity for microalgae processes. This choice resulted in a relatively high consumption of nuclear fuel as the French grid is mainly based on this resource. Similarly, the fossil fuel consumption was relatively high with respect to CED, while other energy resources, notably renewables, were negligible. Obviously, if the process was based in another country, results for CED composition could change drastically as different countries have different energy resources.

In conclusion, the least energy demanding process is BG from algae; this process has interesting potential for both electricity and heat production.

III.7.2. Life Cycle Assessment

The results of the inventory at process level and the corresponding data sets from the Ecoinvent database for the background processes are brought together in see SI III. The results of the LCIA step were obtained at midpoint and endpoint and are extensively presented in see SI III in graphical form. The main results are discussed below.

Figure III.9 shows the endpoint results by energy product (A, B, C) and by area of protection (abscissa). The contributions of different impacts to the endpoint results are shown by the graphical symbol in the histogram bars.

The main contributor for ecosystem quality and concerning human health was the climate change impact. Particulate matter formation also had some influence on the human health category. This result can be correlated with the result on resource depletion, which is dominated by fossil resource utilization. On the other hand, damage by resource depletion was higher for diesel and heat from natural gas - an obvious result given the exclusive use of fossil resources for these types of energy production. Other impacts seem to be negligible with regard to these main components. Nevertheless, they are presented in see SI III.

For fuel production (Figure III.9.A), damage to both ecosystem quality and human health was the worst for BD. For both energy types, damage to human health seemed to be higher than to ecosystems and was due to climate change.

Regarding the environmental damage involved in electricity production (Figure III.9.B), BD showed by far the worst results with respect to the conventional system and BG. Although BG showed the best results for energy balance and CED, here, the biogas process scenario was not better than the conventional one.

For heat production (Figure III.9.C), BG showed the least damage to all three areas of protection, demonstrating an interesting environmental potential for heating production. Here again, BD gave the worst results.

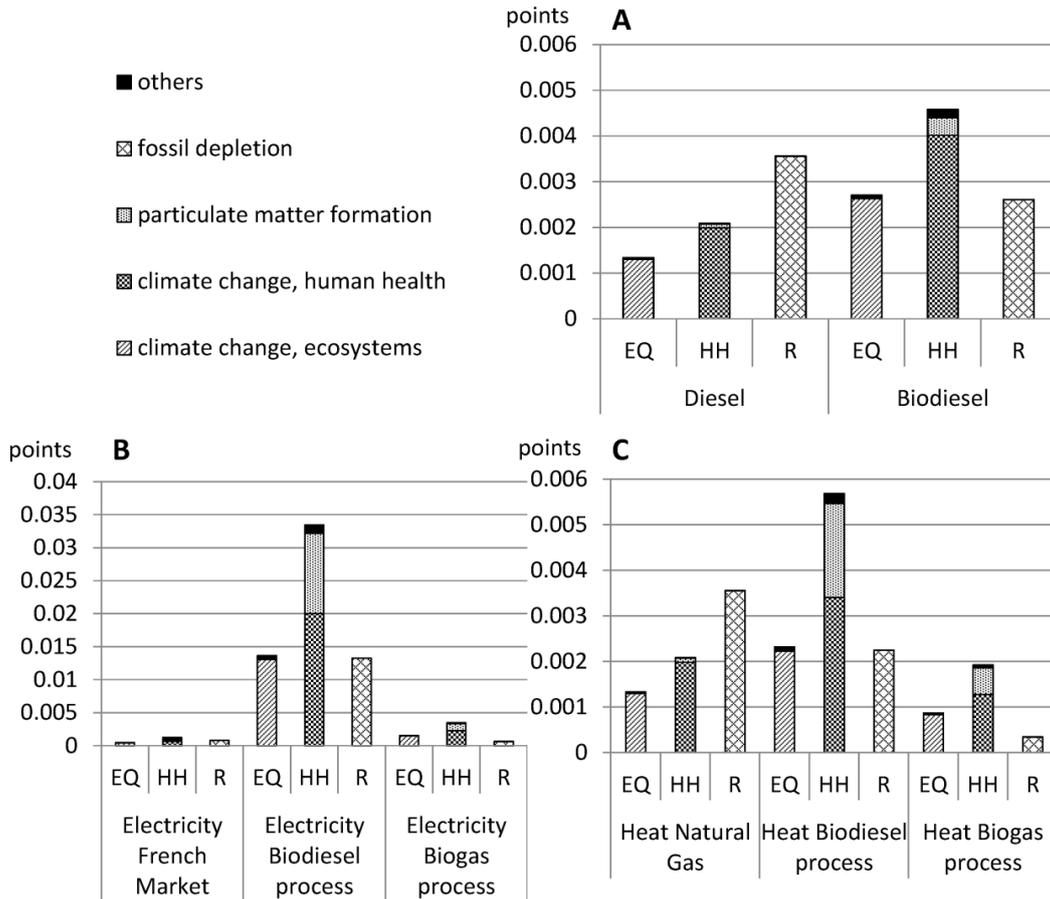


Figure III.9 – Endpoint results: EQ (Ecosystem Quality), HH (Human Health) and R (Resources). (A) Fuel energy production, (B) Electricity production, (C) Heat production.

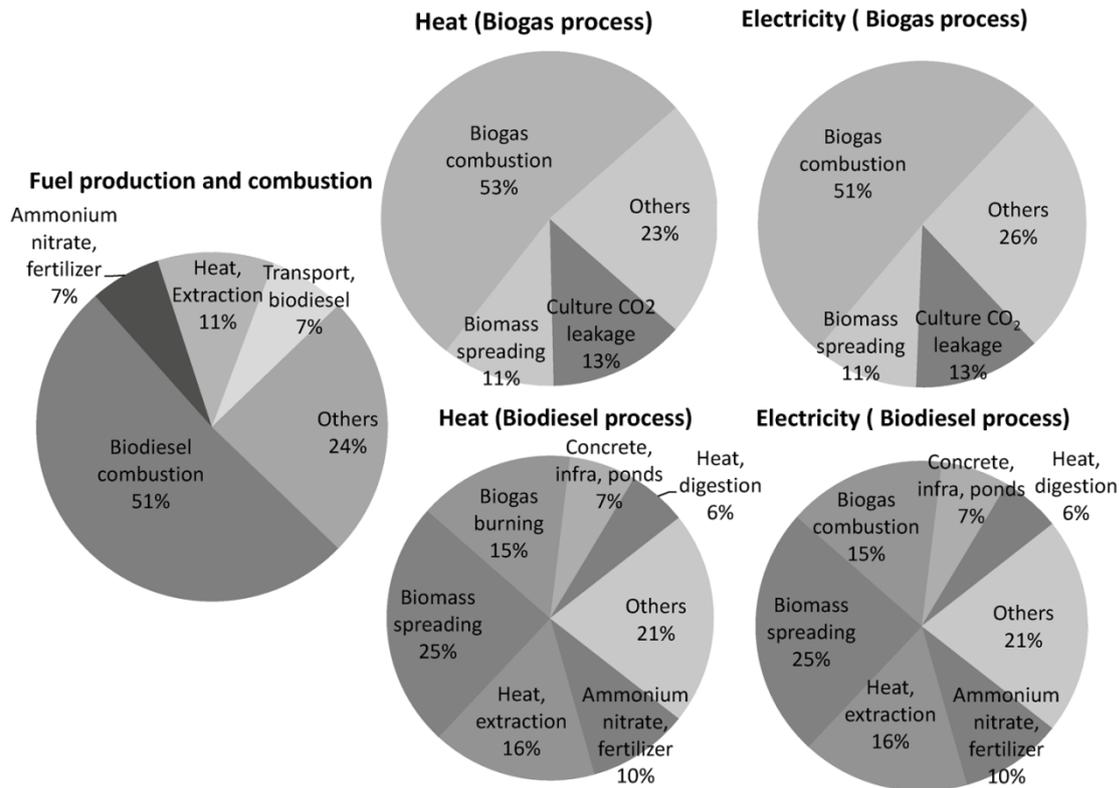


Figure III.10 – Relative contribution of each process to climate change (representation of contributions higher than 5%)

Obviously, climate change is the most important impact contributing to the endpoint damage results for all scenarios. Figure III.10 shows the relative contribution of individual processes to climate change, for each bioenergy product obtained in BD and BG systems. Much of the carbon dioxide contributing to climate change impact was emitted by the combustion of biodiesel and biogas, because microalgae culture was based on fossil carbon dioxide (coming from a thermal power plant using fossil fuels). Microalgae in this system are not a carbon sink but only capture CO₂ for a while, this carbon being released in the energy production process.

For BD, one of the most impacting operations was the supercritical extraction. This was due to the high energy consumption for process operation and additional liquid CO₂ fabrication. In contrast, supercritical transesterification did not present substantial environmental impacts. These results were corroborated by the energy balance and CED results, showing low energy efficiency. Another process contributing to climate change impact was the residual biomass spreading on soils for agriculture. This process generated and released dinitrogen monoxide into the atmosphere, contributing to climate change.

The Renewable Energy Directive (RED) establishes an overall policy for the production and promotion of energy from renewable sources in the EU (RED, 2009). A set of sustainability criteria has been defined to ensure that biofuels and bioliquids are produced and used in ways that guarantee real carbon savings and protect biodiversity. The GHG emission saving from the use of biofuels compared to conventional fuels and energy has to be at least 35% and this will be increased to 50% by 2017 (RED, 2009). The only product that currently respects such conditions is heat from BG, which saves about 36% of GHG. But comparing this process to others using renewable energy revealed that it was not particularly efficient. For example, the process that uses municipal organic waste as raw material for the production of biogas saves about 73% of GHG.

III.7.3. Dynamic LCA - climate change

Dynamic LCI was calculated using the method described in Tiruta-Barna et al. (2016) and the DyPLCA demonstration software (<http://dyplca.univ-lehavre.fr/>). The results were then used to calculate temperature change as a function of time. Temperature change was calculated over the long term (100 years), exceeding the life time of the system, because the effects of a GHG emission show themselves for several years after the emission ceases. Zero time corresponded to the beginning of the operation step of the BD or BG system, considering the construction of infrastructure and equipment to have taken place several years earlier (negative values on the time axis in Figure III.11). Figure III.11 shows the dynamic temperature change over 100 years due to energy production from algae during 10 years. The results are cumulated effects of CO₂, N₂O and CH₄ emitted by the systems studied. However, the contribution of CO₂ was by far the greatest in all the scenarios modelled (see SI III).

The bioenergy production is compared with the conventional energy production in Figures A, B and C.

The contribution of infrastructure construction is very small, then a sharp increase is observed during the 10 years when the process was operating, with a maximum at about 20 years. The delay between the end of the process and the maximum value of temperature change is due to the thermal inertia of various environmental compartments.

The curves of conventional diesel (D) in Figure III.11.A and electricity (FM) in Figure III.11.B are well below the curves for biodiesel and electricity from algae, showing that the conventional scenarios had less effect on climate change. Concerning heat production (Figure III.11.C), the temperature change is quite similar for all production systems.

When the maximum temperatures are compared on the different curves in Figures A, B and C, no significant differences are observed. Maximum temperature values were reached at years 26 and 27 in

all processes. This result gives information about the carbon capture and sequestration capabilities of the systems. A negative temperature variation or a very long delay of the maximum temperature characterizes a carbon sequestration process. The time interval between the input of raw material and the production of energy showed that the microalgae energy cycle was short and did not have any great influence on the climate change response in comparison with conventional processes. Microalgae efficiently captured the carbon dioxide but released it after a fairly short time and, consequently, did not perform carbon sequestration.

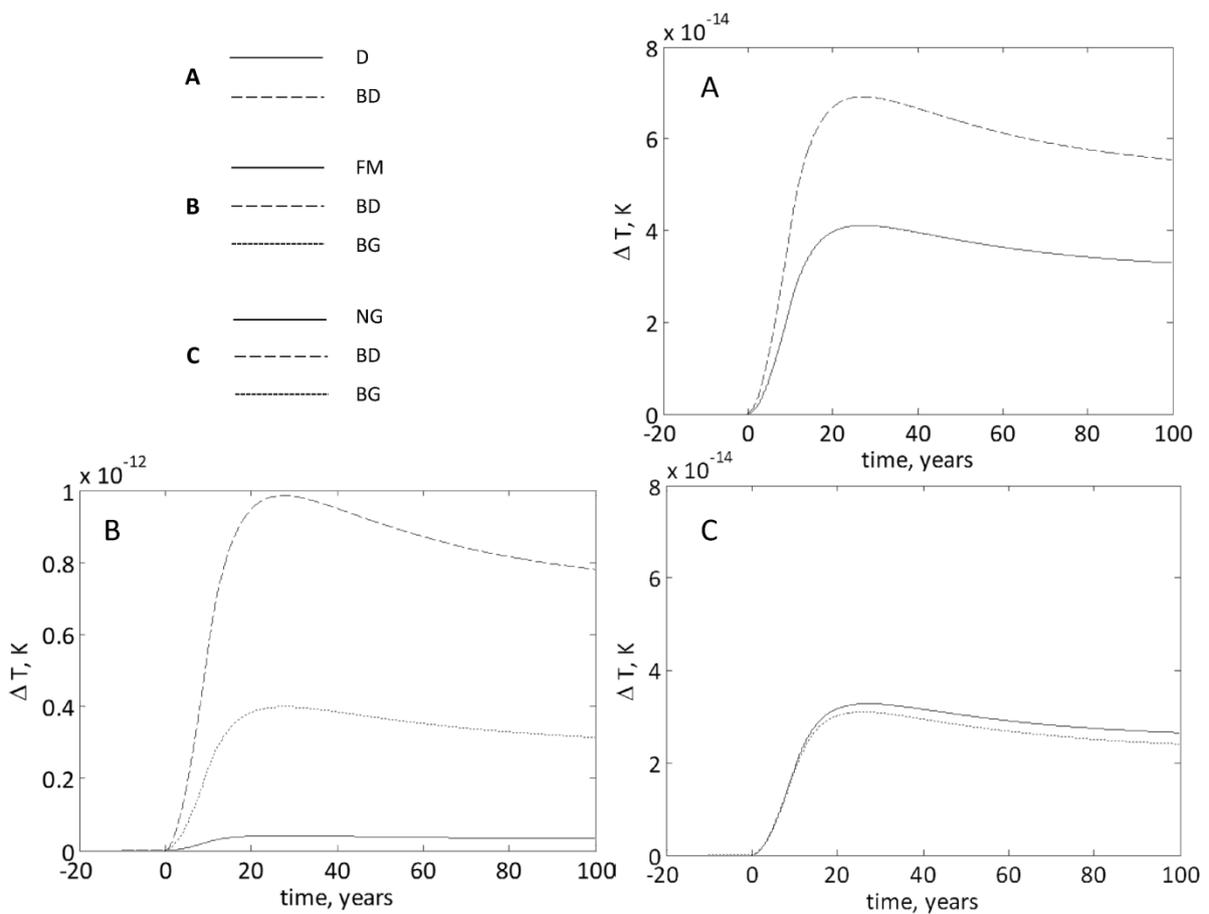


Figure III.11 – Dynamic climate change evaluation for three scenarios: (A) Fuel energy production, (B) Electricity production, and (C) Heat production.

III.8. Case study conclusion

In this study, two ways of transforming microalgae into bioenergy products have been investigated and assessed for their global environmental effects. On the one hand, biodiesel, electricity and heat production was designed through an innovative process (biodiesel production system, BD) using

efficient operations for lipid extraction and transesterification. On the other hand, a very simple process was chosen for transforming biomass into electricity and heat (biogas production system, BG).

Several indicators were calculated for the evaluation of microalgae energy production (biodiesel, heat and electricity) showing different environmental aspects of the processes: energy balance and analysis, LCA and Dynamic LCA.

The results show that technologies for the large-scale production of bioenergy from microalgae still need to be improved and optimized to reduce their impacts on the environment. Biodiesel production did not show efficient energy consumption, mainly because of energy expensive processes. The overall results show better environmental performance for the simplest technology, the BG system. Moreover, heat from the biogas system was the only product that respected RED criteria for bioenergy production.

Concerning the temporal characteristics of the processes, dynamic climate change evaluation showed that the production of bioenergy from microalgae never leads to carbon sequestration.

Algae are often the only possibility to valorise natural sites modified by a previous activity like sea salt extraction, or to draw benefit from natural ponds at the seaside. In these sites, algae growth conditions can be naturally optimal, thus facilitating high productivity. The question of finding the most efficient methods of transformation then arises. The panel of proposed microalgae processes and products is growing but no industrial technologies are currently being developed, except for some alimentary applications. Besides the economic aspects, energy and environmental analysis are crucial for the choice of a sustainable transformation process.

Acknowledgments

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Chapter IV. A dynamic approach for Toxicity impact categories

“How could intelligent beings seek to control a few unwanted species by a method that contaminated the entire environment and brought the threat of disease and death even to their own kind?”

Rachel Carson, Silent Spring

With the advent of industrial revolution and the increase in the rate of industrial development, more and more substances are released in environment. Chemicals which are released in the environment may take different pathways and end up being intake by humans and ecosystems. These substances can have harmful effects depending on the quantity of exposure and the level of hazard that the substance presents.

This chapter has the objective to provide a dynamic method for the assessment of toxicity impact. USEtox[®] model were used as the basis for the new method. The developed method gives results in three categories: freshwater ecotoxicity, human cancer toxicity and human non-cancer toxicity. The calculation of toxicity characterization factor is often the multiplication of three factors: fate, exposure and effect factors. Instead of the use of a fate factor, the new method resolves the Simplebox model in fully dynamic conditions. However, no characterization factors are provided. A current toxicity is calculated as a function of time i.e. the damage produced per unit of time, together with a time dependent cumulated toxicity, i.e. the total damage produced from time zero to a given time span. In order to implement the dynamic impact assessment model, a python program was developed. It is coupled with the DyPLCA inventory results.

The case study presented in this chapter concerns the production of grape. Agriculture activities employ potentially hazardous substances in the different production stages. For example, pesticides are used in the field for the production of grape; also, heavy metals are emitted during the production of raw materials. The temporal behaviour of these substances and the dynamic toxicity categories were investigated.

The framework for the temporal consideration in the toxicity calculation and the case study were published in the journal “Science of The Total Environment”, 599–600 (806-819), doi: 10.1016/j.scitotenv.2017.04.211.

Résumé

Avec le développement industriel, des substances nocives sont de plus en plus libérées dans l'environnement. Les produits chimiques qui sont libérés dans l'environnement peuvent prendre différentes voies et finir par être absorbés par les humains et les écosystèmes. Ces substances peuvent avoir des effets néfastes en fonction de l'exposition et du niveau de danger que présente la substance.

Ce chapitre a pour objectif de proposer une méthode pour le calcul de l'impact toxique en fonction du temps. Le modèle USEtox[®] a servi de base. La méthode développée donne des résultats pour trois catégories: l'écotoxicité dans l'eau douce, la toxicité humaine –cancer et non-cancer. Le calcul du facteur de caractérisation pour la toxicité consiste en la multiplication de trois facteurs caractérisant: le devenir (*fate*), l'exposition et l'effet. La méthode dynamique proposée ne fournit aucun facteur de caractérisation. Les indicateurs proposés sont : le dommage produit par unité de temps, et la toxicité cumulée (le dommage total produit du temps zéro à un point quelconque dans le temps).

Le cas d'étude présenté dans ce chapitre concerne la production de raisins, en raison de l'utilisation importante de pesticides. De plus, des métaux lourds sont émis lors de la production de matières premières utilisées dans le cycle de vie.

L'approche proposée pour le calcul de la toxicité et le cas d'étude ont été publiés dans la revue *Science of The Total Environment*, 599-600 (806-819), doi: 10.1016 / j.scitotenv.2017.04.211.

Le comportement de différentes substances est déterminé par les processus de transport et réactionnels dans l'étape du devenir (dispersion dans l'environnement). Les constantes de ces processus sont rassemblées dans la matrice des constantes K (disponible dans l'outil USEtox[®]). Lorsque des conditions d'état stationnaire sont considérées dans le calcul de la toxicité, comme dans l'ACV conventionnelle, des informations importantes sont perdues ou cachées. L'état d'équilibre dans l'ACV conventionnel conduit à une surestimation des facteurs de caractérisation pour la toxicité, en particulier pour les substances persistantes. Cet aspect de la persistance des polluants n'est pas visible dans les méthodes conventionnelles d'évaluation des impacts de cycle de vie. Il n'est pas possible d'évaluer si le potentiel toxique agit pendant une courte période de temps ce qui affecte les personnes pendant quelques années ou pendant une longue période ce qui affecte plusieurs générations.

Le procédé de "production de raisins" a été modélisé dans SimaPro[®] et la matrice technologique et des interventions environnementales ont été extraites. Les données de SimaPro[®] ont ensuite été utilisées dans DyPLCA avec les paramètres temporels nécessaires.

Les résultats obtenus montrent que la toxicité humaine et l'écotoxicité cumulées sont dominées par les substances inorganiques persistantes, pour lesquelles les méthodes conventionnelles peuvent donner des résultats d'impact surestimés. En outre, plus l'horizon de temps est grand, plus la valeur de la

toxicité cumulée est proche des valeurs de l'ACV conventionnelle. En revanche, les résultats pour la toxicité courante diminuent au cours du temps. En d'autres termes, la population et les écosystèmes sont moins affectés par la pollution résiduelle, mais ils subissent le plus grand dommage dans une période restreinte correspondant à la fin de la vie du système (environ une génération est fortement affectée). Ces résultats soulignent l'importance de l'évaluation d'impact courante comme mesure de l'intensité des dégâts possibles à un moment donné.

Un autre aspect concerne la répartition des différents procédés impliqués dans le cycle de vie de la production de raisins dans le temps. L'approche ICV-EICV dynamique permet d'observer que l'impact principal de la toxicité se produit au moment présent et au futur. L'explication est que tous les produits chimiques et d'autres produits de base sont produits et utilisés pendant la vie des processus de premier plan et aucune infrastructure importante n'a été construite dans le passé. L'impact généré dans le passé par les processus d'arrière-plan est très faible par rapport à l'impact actuel (l'impact passé n'est pas visible sur l'axe de temps négatif, sur toutes les figures). Cependant, les émissions de substances inorganiques provenant des activités passées génèrent un impact persistant visible dans le présent et dans le futur.

D'un point de vue décisionnel, l'évaluation dynamique fournit des informations complémentaires permettant de discriminer des scénarios comparables et de proposer des solutions pour atténuer les impacts. Pour des résultats d'impact conventionnels égaux, le comportement dépendant du temps de la toxicité peut être différent pour les scénarios comparés. Par exemple, le scénario B a plus de contribution de métaux que A (tous égaux, sinon). L'impact à l'échelle de la vie humaine pourrait être moindre dans le cas B car l'horizon temporel est un paramètre très important pour un impact cumulé potentiel en cas de produits chimiques persistants. Le scénario B pourrait être préférable pour de courtes durées comme la durée de vie du vignoble. Des solutions pour changer l'usage des terres pourraient être envisagées afin d'éviter une utilisation sensible (par exemple, pour la production alimentaire) à l'avenir. L'existence de variations avec différentes amplitudes sur les courbes de toxicité suggère que la simulation dynamique peut être utilisée comme outil de prévision pour, par exemple, identifier les situations optimales où certaines activités devraient être (temporairement) arrêtées ou, au contraire, lancées au niveau régional.

Operational integration of time dependent toxicity impact category in dynamic LCA

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Abstract

Life Cycle Assessment (LCA) is the most widely used method for the environmental evaluation of an anthropogenic system and its capabilities no longer need to be proved. However, several limitations have been pointed out by LCA scholars, including the lack of a temporal dimension. The objective of this study is to develop a dynamic approach for calculating the time dependent impacts of human toxicity and ecotoxicity within LCA. A new framework is proposed, which includes dynamic inventory and dynamic impact assessment. This study focuses on the dynamic fate model for substances in the environment, combined with the USEtox[®] model for toxicity assessment. The method takes into account the noisy and random nature of substance emissions in function of time, as in the real world, and uses a robust solver for the dynamic fate model resolution. No characterization factors are calculated. Instead, a current toxicity is calculated as a function of time i.e. the damage produced per unit of time, together with a time dependent cumulated toxicity, i.e. the total damage produced from time zero to a given time horizon. The latter can be compared with the results obtained by the conventional USEtox[®] method: their results converge for a very large time horizon (theoretically at infinity). Organic substances are found to disappear relatively rapidly from the environmental compartments (in the time period in which the emissions occur) while inorganic substances (i.e. metals) tend to persist far beyond the emission period.

Keywords: dynamic Life Cycle Assessment, fate model, toxicity, ecotoxicity

IV.1. Introduction

Life Cycle Assessment (LCA) is a method that calculates potential impacts associated with products, processes and services over their entire life cycle. ISO standards 14040-14044 specify the guide for conducting a LCA study, i.e. the four operational steps: the definition of the goal and scope, the construction of the Life Cycle Inventory (LCI) based on mass and energy balances over the whole system life cycle, the Life Cycle Impact Assessment (LCIA) based on various impact calculation models, and the interpretation step (ISO, 2006a; ISO, 2006b). Currently LCA is the most widely used methodology for evaluating the environmental performance of any anthropogenic system. Its capabilities no longer need to be proved but several limitations have been pointed out by LCA scholars. Among them, the lack of a temporal dimension is intrinsically related to the LCA background. In a state of the art review, Finnveden et al. (2009) argued that “the LCI results are also typically unaccompanied by information about the temporal course of the emission or the resulting concentrations in the receiving environment... The impacts, which can be calculated under such boundary conditions, thus represent the sum of impacts from emissions released years ago, from emissions released today and from emissions released sometime in the future.” Here, two levels can be distinguished, which are related to the LCI and LCIA calculation steps in LCA.

Another time dependent aspect concerns the prospective evolution of systems over time, e.g. changes at the level of technologies or economic sectors. Such issues are resolved either by considering different scenarios at different time periods or by a radically different methodology i.e. Consequential LCA. This aspect is beyond the scope of this work, which focuses on the time dependency of inventory and impacts in Attributional LCA. Including the time dimension in LCA models is a challenge that has been taken up only recently and very little research is currently in progress.

The time dimension in the LCI step has been studied by Beloin-Saint-Pierre et al. (2014). These authors developed an approach called Enhanced Structure Path Analysis, in which environmental interventions (elementary flows, i.e. emissions and natural resources consumed) are distributed over time by considering the convolution product between temporal distributions related to the processes flows and temporal distributions related to elementary flows. However, this method still lacks a full and complete relationship with an LCA database.

To the best of our knowledge, only Tiruta-Barna et al. (2016) have provided a dynamic method for LCI, dealing with the complex supply chain and processes presented in an LCA study and linking the method to traditional LCA tools (databases). It enables easier implementation of temporal characteristics by LCA practitioners. In a recent study, Shimako et al. (2016) applied this method to

bioenergy production from microalgae by calculating temporal LCI and coupling them with a temporal model of climate change.

In fact most studies dealing with temporal aspects in LCA are dedicated to climate change impact. For example, Cherubini et al. (2011) performed a calculation considering dynamic carbon removal by the biomass, which is a step prior to the calculation of the climate change impact. However, dynamic results for midpoint or endpoint climate change impact are not given as the calculated results are integrated in a single unit-based index. Levasseur et al. (2010) and Kendall (2012) studied time dependency in climate change impact by calculating temporal characterization factors (CF) for substances and applying them to dynamic emissions. Nonetheless, the authors focused on the LCIA step and modelled simple systems that did not present a complex network of processes (and emissions) as most LCA studies do. The fixed time step and simple input of data for the LCI did not allow the application of a more complex and complete dynamic LCI in their methods.

In traditional LCA, the mass of the emitted substance is proportionally linked to the impact by using characterization factors as proportionality constants, even though the fate of chemicals in the environment is determined by time-dependent processes such as mass transfer and chemical reactions, which produce non-linear distributions of remaining mass of substances in environment. An infinite time horizon is generally used for the calculation of CF for toxicity impact. This assumption is important for taking all long lasting impacts into account. However, predicting impacts for eternity is also illogical. Also, the consideration of an infinite time horizon may hide the potential impacts occurring over short periods of time in the assessment of a system, because of the different nature of substances considered in the assessment (Huijbregts et al., 2001). The evidence of such shortcomings determined LCA scholars to consider CFs for different time horizons. For toxicity calculations, Huijbregts et al. (2000a, 2000b, 2001) proposed characterization factors based on the USES-LCA model, which comprises fate, exposure and effect calculations. CFs for 20, 100 and 500 years were calculated to be in accordance with the horizon times used in global warming potentials as it was considered that they provided a useful interval for policy decisions.

Another method, proposed by Hellweg et al. (2003), tackles the lack of time influence by applying a discounting method, which considers that toxicity impact diminishes with time. Calculation of time dependent CFs was also the approach proposed by Lebailly et al. (2014) by evaluating the dynamics of substance fate in the environment. They used the USEtox[®] model and calculated the dynamic behaviour of substances for an initial unit load of substance by solving the fate model for these particular conditions. These authors calculated characterization factors at different time steps (starting from the initial emission), and used them for a temporal evaluation of the freshwater ecotoxicity of metals. They applied this method to the use of zinc as a fertilizer in agriculture in order to assess the temporal behaviour of the impact. Although it implements dynamics in the fate calculation for metals,

the study lacks information on organic substances and, also, it does not implement complex, temporal LCIs, which may present dynamic features related to unit processes and supply chains involved in the life cycle of processes.

In conventional LCA, several toxicity models have been developed and used over the years. The Life Cycle Initiative (<http://www.lifecycleinitiative.org/>) program of the United Nations Environment Program (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC) developed the USEtox[®] consensual toxicity model for LCA. USEtox[®] development was based on the comparison of several toxicity models and on experts' recommendations (Jolliet et al. 2006; Ligthart et al. 2004; McKone et al. 2006). USEtox[®] provides toxicity characterization factors for human toxicity and freshwater ecotoxicity that are recommended by LCA scholars.

The objective of this study is to develop a dynamic approach for calculating time dependent toxicity and ecotoxicity impacts within LCA. The USEtox[®] model was chosen and adapted to include the time dimension. In the first part of the paper, the theoretical development is presented. Then, the method is applied to a testbed case, i.e. grape production, in order to emphasize the results of the proposed framework. This testbed case was chosen for a variety of reasons: i) agriculture employs potentially hazardous substances in the different production stages, so a temporal analysis of the LCI and environmental impacts is justified; ii) various substances are emitted into the environment by agricultural operations, i.e. metals and organic compounds with different types of harmful effects on humans and ecosystems.

IV.2. Method

IV.2.1. Toxicity Impact Assessment – USEtox[®] method

This subsection gives a brief presentation of the principles of the toxicity calculation methods in LCA, particularly for the USEtox[®] method. The toxicity calculation methods usually follow the approach used in methods for assessing chemical risk to human and ecosystem health, based on three steps following the causal chain: i) evaluation of the fate of chemicals in the environment, which leads to different concentrations/quantities of substances in different environmental compartments; ii) evaluation of the exposure of humans or ecosystems to a given substance, and iii) the effects that exposure might have on human or ecosystem health (Hauschild et al., 2008). Specific modelling approaches characterize each step, and have given rise to commonly used LCIA methods like IMPACT 2002 (Jolliet et al., 2003; Pennington et al., 2005), ReCiPe (Goedkoop et al., 2009) or USEtox[®] (Hauschild et al., 2008). All the methods cited are based on a similar framework consisting of the calculation of characterization factors for substances as the result of multiplying a fate factor, an

exposure factor and an effect factor together, each of them being the result of one of the three corresponding modelling steps cited above (Huijbregts et al, 2005a and 2005b).

Rosenbaum et al. (2007) proposed a framework in which the characterization factor was calculated as the product of matrices representing fate, exposure and effect factors:

$$\mathbf{CF}_s = \mathbf{EF}_s \cdot \mathbf{XF}_s \cdot \mathbf{FF}_s \quad \text{Equation IV.1}$$

where the index s represents the substance of concern, \mathbf{CF} is the characterization factor vector in which each row represents a compartment, \mathbf{FF} is the fate factor matrix representing the environmental removal and transport processes of a certain substance in the different environmental media, \mathbf{XF} is the exposure factor matrix representing the increase in human consumption of a particular substance based on the increase of the substance concentration in a certain medium (for human toxicity) or the bioavailability of a certain substance (for ecotoxicity), \mathbf{EF} is the effect factor matrix, which express the effect on humans or ecosystems per unit of concentration (Rosembaum et al., 2007). The USEtox[®] calculation tool (available at <http://www.usetox.org/>) is based on this flexible matrix algebra.

Finally, for toxicity impact calculations, the characterization factor is multiplied by the aggregated environmental intervention of certain substance over its entire life cycle:

$$n_{s,i} = \mathbf{CF}_{s,i} \cdot \mathbf{g}_{s,i} \quad \text{Equation IV.2}$$

where index i represents the emission compartment, \mathbf{g} represents the environmental intervention (aggregated mass, which is the result of the LCI step) and n is the toxicity impact value for a certain substance s emitted in compartment i .

IV.2.1.1. Fate modelling

Fate modelling uses a concept developed in the 1980s (described in many publications, e.g. Mackay, 2002; Van de Meent, 1993), which considers the environment as connected, well mixed, homogeneous boxes (named environmental media or compartments). The mass/concentration of a substance varies with time due to transport between compartments, reaction processes (e.g. degradation), and removal (immobilization in different media). In this model, the mass balance of a substance in the environment is described by a system of ordinary differential equations (ODE):

$$\frac{dm_s}{dt} = \mathbf{K}_s \mathbf{m}_s + \mathbf{g}_s \quad \text{Equation IV.3}$$

where \mathbf{K} is the square matrix of rate constants (related to removal, degradation and transport processes) in each compartment i (day^{-1}), \mathbf{m} is the mass vector of substance s in the respective environmental compartments (kg), \mathbf{g} is the vector of emission flows in each compartment (kg day^{-1}), t is time.

The nested multimedia fate concept is also used in LCIA methods but in the very simplified condition of equilibrium or steady state. Physically the fate factor (day) represents the persistence of a chemical in the environment. It is mathematically defined as the resident mass (kg) in a certain compartment per unit of constant flow ($\text{kg}\cdot\text{day}^{-1}$) emitted into the environment. In terms of the ODE system (Equation IV.3) that signifies no variation of the concentrations/masses, in all compartments:

$$\frac{dm_s}{dt} = 0 = \mathbf{K}_s \mathbf{m}_s + \mathbf{g}_s \quad \text{then} \quad \mathbf{FF}_s = \frac{\mathbf{m}_s}{\mathbf{g}_s} - \mathbf{K}_s^{-1} \quad \text{Equation IV.4}$$

The USEtox[®] 2.0 model is based on the steady-state condition described by Equation IV.4. The following scales and compartments are defined (Hauschild et al., 2008): global scale (air, freshwater, ocean, natural soil, agricultural soil), continental scale (rural air, freshwater, sea water, natural soil, agricultural soil), local scale (urban air, household indoor air and industrial indoor air).

IV.2.1.2. *Exposure modelling in USEtox[®]*

The exposure factor represents the relationship between the quantity of substance present in a certain compartment and its intake by humans. It can be divided into direct (i.e. direct consumption of an environmental compartment) and indirect exposure (e.g. meat, dairy produce, vegetables, etc.), represented respectively by Equation IV.5 and 6 (Rosebaum et al., 2007).

$$XF_{s,xp,i}^{direct} = \frac{IR_{xp,i} \cdot P}{\rho_i \cdot V_i} \quad \text{Equation IV.5}$$

$$XF_{s,xp,i}^{indirect} = \frac{BAF_{s,xp,i} IR_{xp,i} \cdot P}{\rho_i \cdot V_i} \quad \text{Equation IV.6}$$

where XF_{direct} (day^{-1}) represents the average direct intake rate of the polluted medium i via direct ingestion. The parameter ρ is the bulk density of medium i ($\text{kg}\cdot\text{m}^{-3}$), V (m^3) is the volume of medium i

related to the exposure pathway x_p , IR ($\text{kg}\cdot\text{day}^{-1}$) is the ingestion rate of medium i via exposure pathway x_p at population level and P is the population head count. For XF_{indirect} (day^{-1}), IR ($\text{kg}\cdot\text{day}^{-1}$) represents the individual intake rate of food substrate correlated to pathway x_p and $BAF=C_{x_p}/C_i$ ($\text{kg}\cdot\text{kg}^{-1}$) is the bioaccumulation factor (the steady state concentration ratio between food substrate corresponding to exposure pathway x_p and compartment i). For ecotoxicity, the exposure factor represents the relationship between the quantity of the substance in environmental compartments and its available fraction (truly dissolved fraction) (Rosenbaum et al., 2011).

IV.2.1.3. *Effect modelling in USEtox[®]*

The effect factors represent the relationship between the intake quantity and the possible negative health effect of substances for living organisms. The effect factor for humans (cancer and non-cancer effects) can be calculated by Equation IV.7. A linear dose-response function was assumed for each disease endpoint and intake route (Rosenbaum et al., 2011).

$$EF_s = \frac{0.5}{ED50_s} \quad \text{Equation IV.7}$$

where EF is the effect factor for humans ($\text{cases}\cdot\text{kg}^{-1}$) for substance s , $ED50$ is the lifetime daily dose resulting in a probability of effect of 0.5 (Henderson et al., 2011).

The effect factor for ecotoxicity ($\text{PAF}\cdot\text{m}^3\cdot\text{kg}^{-1}$) represents the change in the Potentially Affected Fraction (PAF) of species due to change in concentration:

$$EF_s = \frac{0.5}{HC50_{s,EC50_s}} \quad \text{Equation IV.8}$$

where $HC50$ is defined by the hazardous concentration at which half of the target population is exposed above its $EC50$ (concentration for which 50% of the population is affected) (Henderson et al., 2011).

IV.2.2. *Time consideration in toxicity impact assessment*

Among the factors included in a toxicity calculation, the fate is the one for which the dynamic aspects are the most evident. It is well-known that the fate of substances in the environment depends on their nature. Organic substances can be degraded by the environment, which leads to their disappearance. On the other hand, inorganic substances (metals) tend to be persistent and stay in different

compartments for a long time (Hauschild et al., 2008). It is important to account for the dynamic behaviour of substances in the environment by considering all the phenomena involved, such as mass transfer, degradation of substances, removal, etc., as described by the mass balance system of equations (Equation IV.3). Therefore, considering the steady state condition, as is the case in conventional LCA, may lead to loss of consistency. The dynamic mass balance model provided, once adapted, can be resolved by numerical methods. It should be noted that the environmental intervention g (Equation IV.3) represents emission flows with complex temporal behaviour which requires a rigorous resolution approach. The input data g can be defined as a time dependent function in an analytical manner or as numerical values at given times. Moreover, the rate-constants matrix K contains values of different orders of magnitude (in day^{-1}) which signify the combination of slow and rapid kinetics, with very different slopes. This condition imposes the use of finite difference solvers with a very narrow discretization of the time dimension that has to be investigated, or solvers with variable, adaptive, time steps. In this work, the Python odeint integrator (SciPy Python library) was employed to solve initial value problems. It automatically switches between an Adams predictor-corrector method for non-stiff problems and a backward differentiation formula method for stiff problems. In this work, the mass balance model in Equation IV.3 was used with the specific data provided by the USEtox[®] model, i.e. kinetic constants, exposure and effect factors for the defined environmental scales and compartments.

The result of the ODE is a vector of 13 elements that represents the current masses of substance s in each compartment i at a specific time t . By the end of the calculation, a mass vector (13 values corresponding to each compartment) is obtained for each discrete time value. For the toxicity results, following the matrix approach proposed by Rosenbaum et al. (2007), each mass vector is multiplied by the exposure matrix (XF) and effect matrix (EF):

$$n_{human,s}(t) = \mathbf{m}_s(t) \times \mathbf{XF}_{human,s} \times \mathbf{EF}_{human,s} \quad \text{Equation IV.9}$$

$\mathbf{n}_{human}(t)$ is the vector that represents human toxicity (cancer and non-cancer, cases.day^{-1}) for a certain substance s in different compartments, at a given moment t in time.

$$n_{eco,s}(t) = \mathbf{m}_s(t) \times \mathbf{XF}_{eco,s} \times \mathbf{EF}_{eco,s} \quad \text{Equation IV.10}$$

$\mathbf{n}_{eco}(t)$ represents the ecotoxicity, $(\text{PAF.m}^3.\text{day}).\text{day}^{-1}$, due to an emission into a specific compartment for a certain substance s at a given moment in time t .

The result for the aggregation of all substances s and compartments i , for a given time t , is given by Equation IV.11 and 12 for human and eco-toxicity, respectively.

$$n_{human}(t) = \sum_s \sum_i n_{human,s,i}(t) \quad \text{Equation IV.11}$$

$$n_{eco}(t) = \sum_s \sum_i n_{eco,s,i}(t) \quad \text{Equation IV.12}$$

The cumulated values, $n_{human,cumul}$ (cases) and $n_{eco,cumul}$ (PAF.m³.day), for human toxicity and ecotoxicity can be calculated using equations V.13 and 14 respectively.

$$n_{human,cumul} = \int_{t=t_0}^{TH} n_{human}(t) dt \quad \text{Equation IV.13}$$

$$n_{eco,cumul} = \int_{t=t_0}^{TH} n_{eco}(t) dt \quad \text{Equation IV.14}$$

where t_0 represents the time of the first emission released into the environment, TH is the time horizon for which the impact is investigated.

The objective of this work is the adaptation of USEtox[®] steady-state model for a dynamic representation of the chemicals fate. The USEtox[®] 2.0 physical parameters were used without modifications. Nevertheless, the authors are aware about the limitations and simplifications in the LCIA methods. The chemicals fate in environment reveals much more complexity than that described by the multimedia fate models used in LCIA. Examples of influence factors are: local characteristics of environmental media which depend, besides the geological parameters, on specific climate factors and biota (e.g. Hertwich, 2001a; Daly and Wania 2004), chemical speciation and its dependence on the above cited factors (Gandhi et al, 2011), and global modifications at long term of all these parameters. Obviously, a more accurate representation should consider time and region dependent transport and kinetic parameters in a more complex nested multimedia.

Dynamic aspects can also be found in exposure and effect factors. Exposure of organisms to a specific pollutant during a long time period may lead to high mortality and morbidity in the first years. However, it may also lead to a genetic adaptation of organisms or a structural change in the species composition of the ecosystem, decreasing mortality and morbidity (Heijungs et al., 2004). Temporal aspects may also occur in the indirect intake of pollutants via the food chain, which normally delays the moment of pollutant intake with respect to the current pollution state. However, these processes

are not considered in this study as the prediction of such behaviour is complex and uncertain, and remains beyond the scope of this work. Here, the conventional exposure model (Equation IV.5, 6), and linear dose-response functions (Equation IV.7, 8) are used.

IV.2.3. Integration in a Dynamic LCA framework - DyPLCA

Introducing the time dimension into the LCIA step, in particular for toxicity calculation, is not sufficient to provide a relevant temporal assessment in LCA. A reliable time dependent LCI must be set up. Recently, a novel conceptual and computational framework for including time dependency in LCI was proposed by Tiruta-Barna et al. (2016). This method considers the temporal behaviour of the foreground processes and of the supply chain. It takes temporal characteristics such as residence time of processes, lifetime of infrastructures, delivery scheduling of products and latent time in the supply chain into account (more details in the SI IV.6). Each process is characterized by a production flow function and an emission flow function. In order to distribute the environmental interventions over time, the life cycle network of processes is described as a graph in which the nodes represent the processes and the arcs the exchange of products. For the computation of the time-resolved environmental interventions, a tracking (graph search) algorithm is implemented in a Web software named DyPLCA (<http://dypca.univ-lehavre.fr/>). In terms of results, the new approach provides time dependent LCI expressed as: i) a time function for individual emissions (or resource consumption) for individual processes, ii) an aggregated time function for a given environmental intervention. The results are obtained in the form of numerical data for discrete time values, over the time span of the life cycle under study (i.e. past activities in background, present and future activities for fore- and background processes, e.g. 100 years). The proposed approach and tool are generic and fully compatible with all dynamic LCIA methodologies and were recently used with a dynamic climate change approach by Shimako et al. (2016).

Three different tools were interconnected in order to obtain a modelling and computational framework for dynamic toxicity in LCA (Figure IV.1). SimaPro[®] LCA software was used for the traditional LCI resolution. This software delivers the LCI results in matrix form: a technological matrix and an environmental intervention matrix (emissions by compartments and processes). Those results were then used in the DyPLCA platform together with all the temporal characteristics of processes and supply chains (defined by the practitioner prior to calculation). This tool delivered a time vector and the associated emissions vector (kg.day⁻¹) in different environmental compartments, which were then used in the dynamic toxicity model proposed by this study. A Python program treats data interpolation, choice of time step for calculation, and sends the data to the ODE solver together with all the necessary USEtox[®] parameters, then retrieves and treats the toxicity results. The complete dynamic framework was applied to a testbed case.

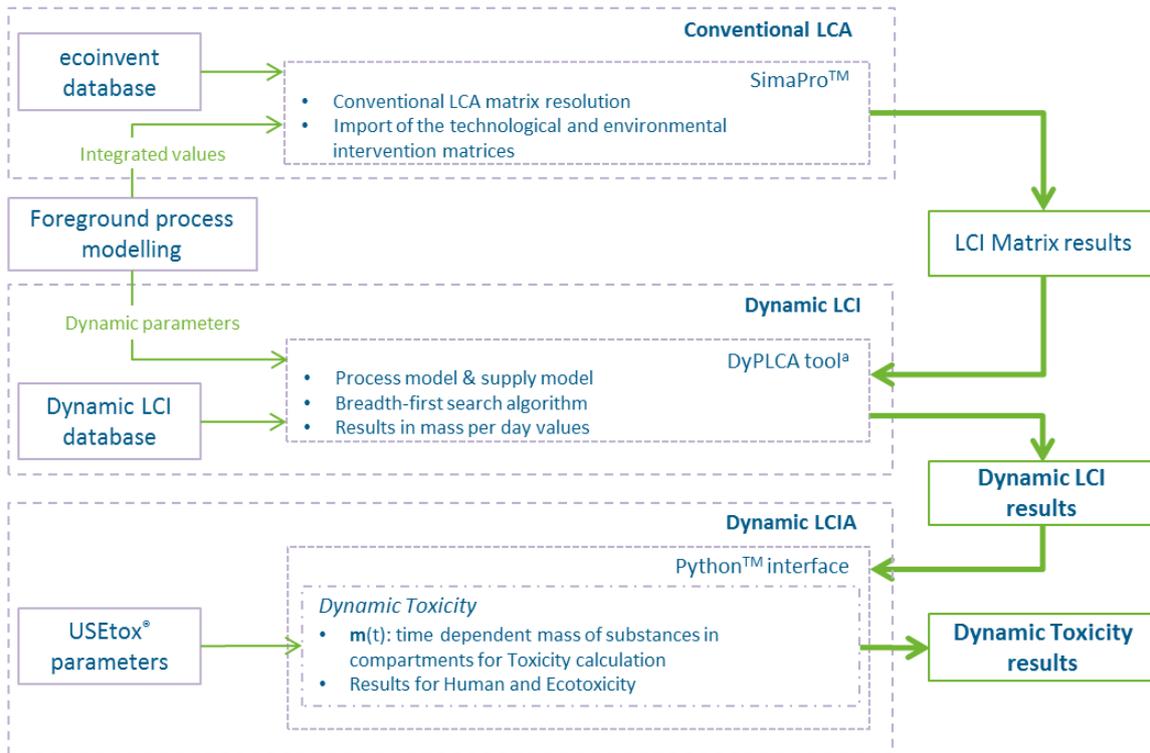


Figure IV.1 – General framework for the calculation of a dynamic LCA

IV.2.3.1. *Practical application to a testbed case*

The process of “grape production, GLO” in version 3.2 of the ecoinvent database was considered as testbed case in order to exemplify the dynamic evaluation of toxicity using USEtox[®]. Conventional and dynamic LCA were performed and the results were compared.

IV.2.3.2. *Conventional Life Cycle Assessment of grape production*

Goal and scope definition

From an LCA point of view, the objective of this study is to evaluate the toxicity impacts for the production of 1 kg of grapes (the functional unit). Cradle to gate boundaries are considered following the ecoinvent dataset “grape production, GLO” with attributional allocation.

This dataset (presented in SI- IV.3) covers the processes starting from the initial maintenance of the vineyard just after the previous crop, to the harvest and storage of the grapes produced, and includes fertilizer acquisition and application, pesticide acquisition, electricity use and irrigation. More details can be found in Stoessel et al. (2012).

Life cycle inventory

Global geography (GLO) is the only geography available in ecoinvent 3.2 and was chosen for this study. For this reason, several improvements were necessary to match agricultural practices better at regional scale. Regarding organic substance emissions, few substances could be found in the “grape production” dataset. The emissions were accounted for in the process “pesticides, unspecified” in the technosphere. However, some important pesticides currently used in agriculture were not considered. In Europe, France was the main agricultural pesticides producer in 2013. It ranked second for absolute sales of pesticides, with a share of almost 19% in 2014, and ranked third for grape production (Eurostat, 2016). In this sense, the French market was chosen to represent the quantities of pesticides to be taken into account. For this purpose, the dataset “pesticide, unspecified” and the emission “pesticide, unspecified” were modified to fit the values available for the French market (MEDDE, 2016 - French national sales data base - provides the French market distribution for pesticides). For this study, only 34 compounds were selected, corresponding to 55% of the French market in 2014 (Table IV.1).

Table IV.1– Share of pesticides in French market - substances that contribute more than 0.5% to the market (classified by their abundance in 2014).

Substance	2013	2014	Substance USEtox[®] name	Substance ecoinvent name
Sulfur	19.7%	17.9%	n.a.	Sulfur
Glyphosate	14.3%	13.4%	Glyphosate	Glyphosate
Mancozeb	5.24%	7.02%	Mancozeb	Mancozeb
Metam-sodium	3.12%	3.31%	Methyldithiocarbamic acid, Na salt	Metam-sodium
Prosulfocarb	2.16%	3.27%	Prosulfocarb	
s-Metolachlor	0.00%	2.89%	Metolachlor	Metolachlor
Chlormequat	2.78%	2.84%	Chlormequat	Chlormequat
Isoproturon	2.10%	2.48%	Isoproturon	Isoproturon
Folpet	2.49%	2.31%	Folpet	Folpet
Chlorothalonil	2.12%	2.03%	Chlorothalonil	Chlorothalonil
Iron sulphate	2.17%	1.98%	n.a.	n.a.
Paraffin oil	1.49%	1.69%	n.a.	n.a.
Chlorotoluron	1.89%	1.63%	Chlortoluron	Chlorotoluron
Metiram	1.65%	1.55%	Metiram	Metiram
Pendimethalin	1.28%	1.32%	Pendimethalin	Pendimethalin
Copper from copper sulphate; Copper from tetracopper	1.39%	1.21%	Cu(II)	Copper

tricalcium sulphate				
Metaldehyde	1.72%	1.18%	Metaldehyde (tetramer)	Metaldehyde
Aclonifen	1.30%	1.16%	Aclonifen	Aclonifen
Dimethenamid	1.08%	1.09%	Dimethenamid	Dimethenamid
MCPA	1.36%	1.05%	MCPA - Sodium salt	MCPA
Metazachlor	1.25%	1.00%	Metazachlor	Metazachlor
Napropamide	1.00%	0.91%	n,n-Diethyl-2-(1-naphthalenyloxy)propanamide	Napropamide
2,4-d	0.96%	0.89%	2-(2,4-dichlorophenoxy)acetic acid	2,4-D
Prochloraz ; Prochloraz manganese	1.02%	0.86%	Prochloraz	Prochloraz
Prothioconazol	0.96%	0.84%	n.a.	Prothioconazol
Tebuconazole	0.81%	0.80%	Tebuconazole	Tebuconazole
Metamitron	0.85%	0.78%	Metamitron	Metamitron
Pronamide	0.64%	0.73%	Pronamide	Pronamide
Amitrol	0.64%	0.68%	Amitrole	
Mineral oils	0.30%	0.61%	n.a.	n.a.
Copper from copper hydroxide	0.72%	0.61%	Cu(II)	Copper
Thiram	0.64%	0.55%	Thiram	Thiram
Imidacloprid	0.45%	0.52%	Imidacloprid	Imidacloprid
Boscalid	0.64%	0.52%	n.a.	n.a.

n.a. = not applied

LCIA

The application case focuses on human toxicity and ecotoxicity impacts generated by the substances emitted in the life cycle. The USEtox[®] 2.0 method was used for the conventional LCIA. In conventional LCIA toxicity impacts are calculated in steady-state condition, i.e. for an infinite time horizon.

IV.2.3.3. Dynamic toxicity assessment

Dynamic LCI

As noted in subsection 2.3, a certain number of temporal parameters are needed in order to compute dynamic LCI. The duration of one production cycle of grape is taken to be 12 months in permanent

culture, the period defined as starting in January of each year. The lifetime of the production field is regarded as 25 years as recommended by Bordelon et al., 2000. The main application of pesticides takes place between April and July and they are applied every 7-14 days in general (Bordelon et al., 2000). For this study, an interval of 7 days was chosen. Direct emissions (i.e. N₂O) of soil fertilization to the air are considered to occur continuously during the production cycle. Fertilizers and pesticides are considered to be delivered to the process of grape production twice a year. The process related to the application of fertilizer, “fertilizing, by broadcaster”, has the same temporal characteristics as the pesticides application. For this study, the harvest month was set as September, as it usually occurs between August and October. The grape produced is stored for 2 months (Nemecek and Kägi, 2007) after the harvest and irrigation was considered to be continuous between April and October.

Based on this information, the temporal characteristics of processes involved in the life cycle of grape production were defined in the dynamic LCI method proposed by Tiruta-Barna et al. (2016) (listed in SI-IV.6). The inventory quantitative data fromecoinvent and the temporal parameters were used with the DyPLCA tool in order to build the temporal LCI.

Dynamic LCIA

Here only toxicity and ecotoxicity impacts were evaluated using the dynamic approach developed in section 2.2.

IV.3. Results and Discussion

This section is structured in two sub-sections. In the first part the feasibility of the new method and the comparison with the conventional method is discussed through two simple examples. The second part presents and discusses the results for the testbed case.

IV.3.1. Discussion of the dynamic toxicity approach

An organic substance (chloroform) and an inorganic one (mercury) were analysed here. For each substance, an emission was considered over 20 years in the agricultural soil compartment, described by a simple step behaviour (Figure IV.2.A): 0.04 kg.year⁻¹ constant flow during the first 10 years, then a constant flow of 0.06 kg.year⁻¹ between years 10 and 20. The total mass of emission is 1kg (time integral of the emission flow).

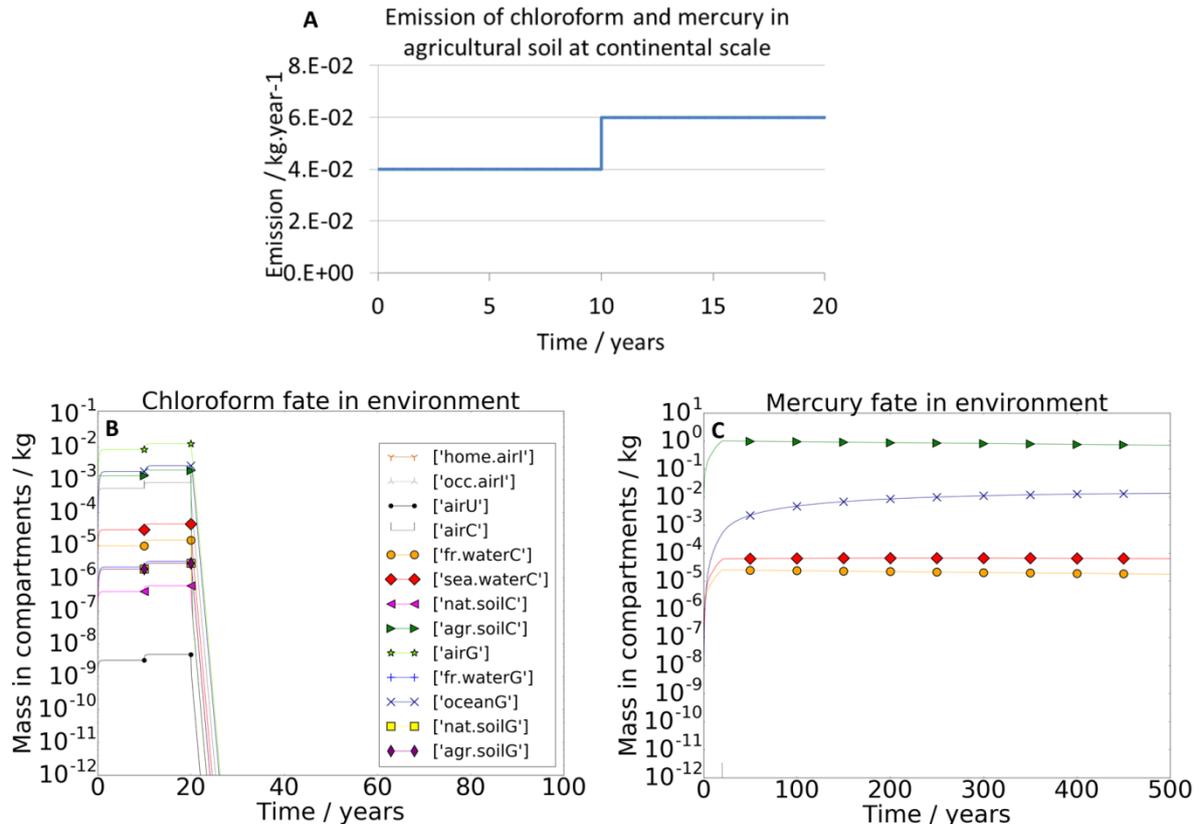


Figure IV.2 – (A) Emission profile of chloroform and mercury into agricultural soil at continental scale. (B) Chloroform fate in environment over 100 years and (C) Mercury fate in environment over 500 years. Legend: home.airI = household indoor air, occ.airI = industrial indoor air, airU = urban air, airC = continental rural air, fr.waterC = continental freshwater, sea.waterC = continental sea water, nat.soilC = Continental natural soil, agr.soilC = Continental agricultural soil, airG = global air, fr.waterG = Global freshwater, oceanG = ocean, nat.soilG = Global natural soil, agr.soilG = Global agricultural soil.

In order to convert the dynamic emission into a dynamic toxicity calculation, the first step is to calculate the fate of the substance. Figure IV.2.B and Figure IV.2.C show the current mass of chloroform and mercury in the environmental compartments, for a calculation time of 100 years and 500 years respectively. The very different behaviours found for the two substances depend on the different mechanisms included in the USEtox[®] model. Accordingly, the remaining mass of chloroform drops considerably after the last emission around year 25. For non-persistent organic substances, kinetics of removal and degradation usually present a high order of magnitude, which explains the fast depletion of chloroform in the environment. The dynamics of mercury removal in the environment is still slow and the sum of the remaining mass of mercury in all compartments at year 500 represents

71% of the total emitted mass. It should be noted that, after an accumulation during the emission period, the mass decreases in the emission compartment (agricultural soil) while it increases in others, e.g. ocean. All transfer and removal processes are slow, explaining the slow, long-term evolution of mercury quantities.

Figure IV.3 shows the current dynamic toxicity impacts ($n_{\text{human}}(t)$, $n_{\text{eco}}(t)$ – Equation IV.11, 12), calculated for 100 years in case of chloroform and for 500 years in case of mercury.

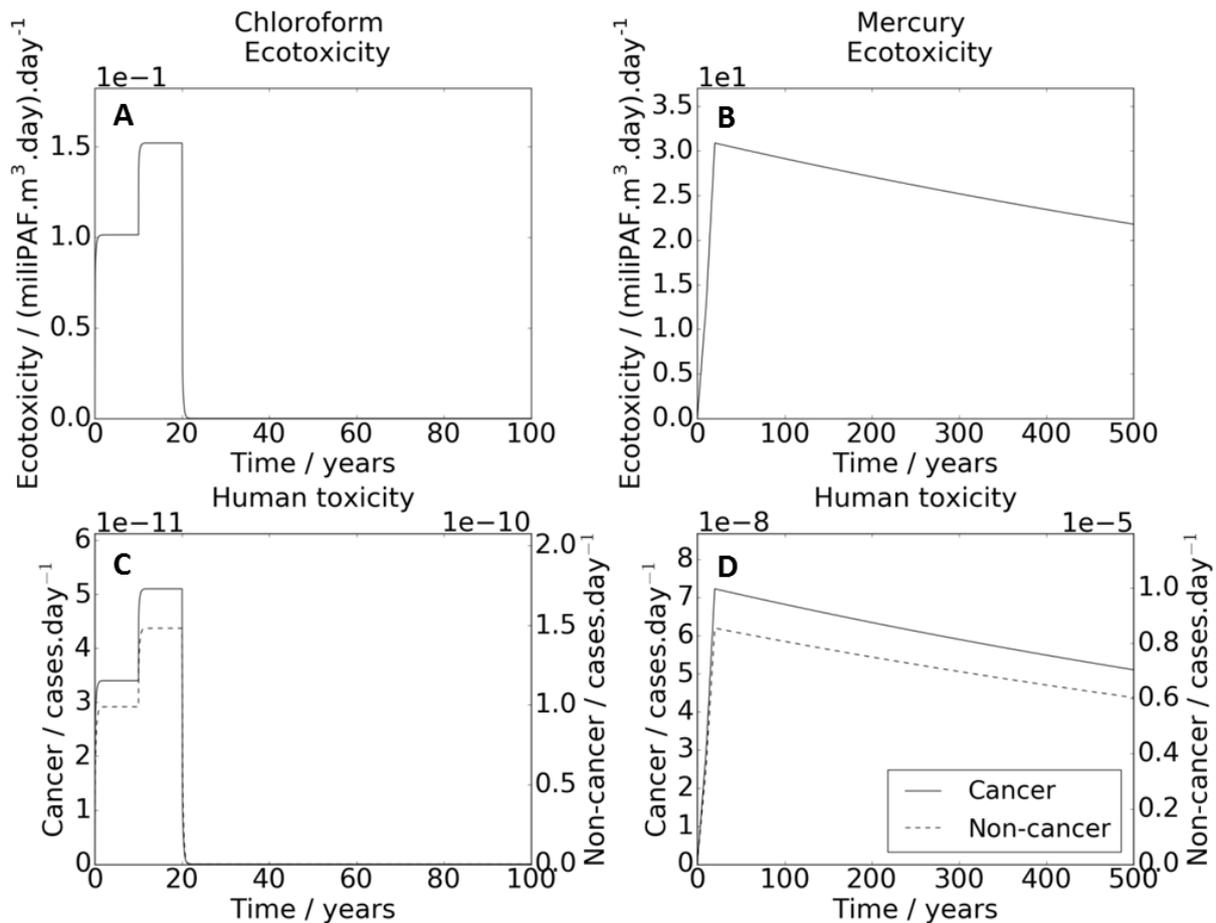


Figure IV.3 – Current dynamic toxicity impacts calculated for 100 years in case of chloroform and for 500 years in case of mercury. Ecotoxicity (n_{eco}) for chloroform (A) and mercury (B); Human toxicity (n_{human}) for chloroform (C) and mercury (D).

For both substances, the shapes of ecotoxicity (Figure IV.3.A and Figure IV.3.B) and human toxicity curves (Figure IV.3.C and Figure IV.3.D) are similar to those obtained for the mass in the fate calculation (Figure IV.2), which is explained by the fact that the dynamic aspects are related only to the fate step. Exposure and effect steps, being considered independent of time, are characterized by constant values. In case of chloroform, the value of toxicity drops considerably after about 20 years

from the first emission, leading to the conclusion that toxicity impact occurs for the time frame in which the emissions exist.

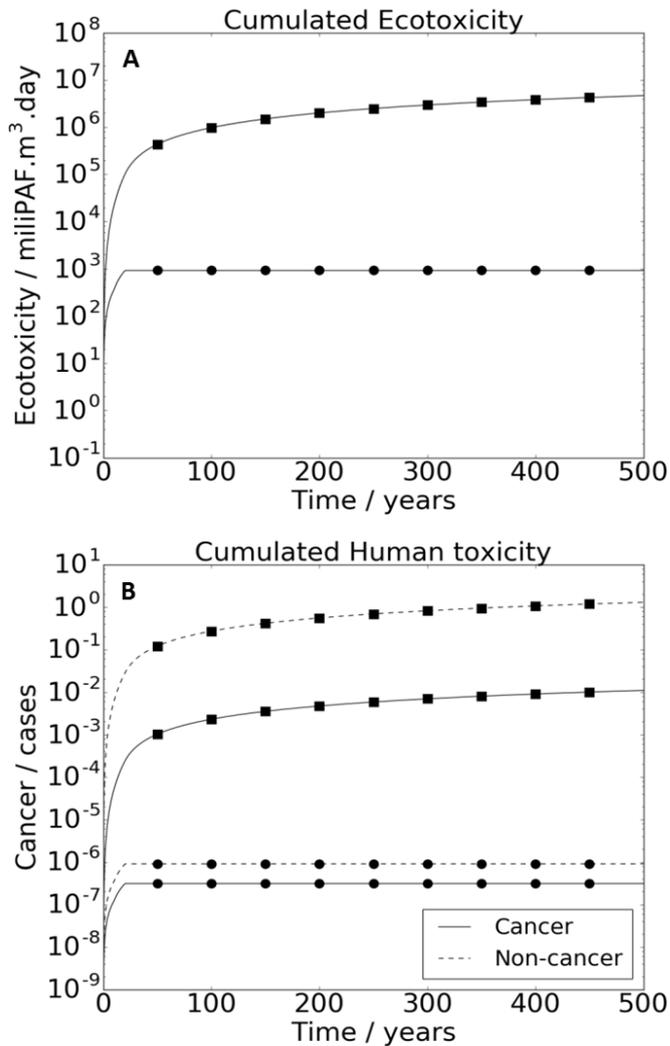


Figure IV.4 – Cumulated dynamic toxicity calculated over 500 years for chloroform emission (●) and mercury emission (■) (mission during 20 years). Ecotoxicity $n_{eco,cumul}$ – A; Human toxicity $n_{human,cumul}$ – B

Figure IV.4 shows the values of cumulated toxicity (Equation IV.13, 14), for chloroform and mercury, for a time horizon of 500 years. This kind of result should be interpreted as the total impact generated from time zero to a given time horizon TH, and, for sufficiently large TH, the results should be similar to those calculated by the conventional method (USEtox[®], infinite TH).

In case of chloroform (non-persistent substance) ecotoxicity and human toxicity stabilize after the end of the emission period. In case of mercury, the cumulated toxicity is still increasing significantly as the substance remains in the environment for a long period. In conclusion, the dynamic method demonstrates that mercury generates toxicity in the long term as a consequence of its persistence in the environment, with a variable intensity culminating at the end of the emission period (maximum of mass accumulation in the emission compartment).

Table IV.2 shows the conventional toxicity results and the cumulated values (obtained for 100 and 500 years integration time) obtained from the dynamic toxicity model, for both analysed substances. In case of chloroform, the values found through the dynamic evaluation are similar to those obtained from the conventional (infinite time horizon) method, thus validating the structure of dynamic calculations for toxicity. In the case of mercury, the results for 500 year time horizon are lower than the conventional results. This can be explained by the fact that the chosen time horizon might not be sufficient to reach the complete removal of the substance. However, it can be noted that the value tends to the traditional toxicity value when TH is increased.

Table IV.2 – Toxicity results for the emission of chloroform and mercury.

		Conventional	Dynamic 100 years	Dynamic 500 years
Mercury	Remaining mass (kg)		9.4E-01	7.2E-01
	Ecotoxicity, cumulated (miliPAF.m ³ .day)	1.6E+07	9.8E+05	4.7E+06
	Cancer toxicity, cumulated (cases)	3.7E-02	2.3E-03	1.1E-02
	Non cancer toxicity, cumulated (cases)	4.3E+00	2.7E-01	1.3E+00
Chloroform	Remaining mass (kg)		0.0E+00	0.0E+00
	Ecotoxicity, cumulated (miliPAF.m ³ .day)	9.3E E+02	9.3E+02	9.3E+02
	Cancer toxicity, cumulated (cases)	3.1E-07	3.1E-07	3.1E-07
	Non cancer toxicity, cumulated (cases)	9.0E-07	9.0E-07	9.0E-07

As a general conclusion, the behaviour of different substances is determined by the transport and reaction processes in the fate step. The rate constants of these processes are gathered in the constants matrix K (available with the USEtox[®] tool). All of them are compartment and substance sensitive. When steady state conditions are considered in the toxicity calculation, important information is lost or hidden. The equilibrium state in conventional LCA leads to overestimation of CFs for toxicity, especially for persistent substances. This aspect of the pollutant persistence and its associated toxicity

is not visible in conventional LCIA methods, i.e. it is not possible to evaluate if toxicity acts for a short period affecting people for several years (as in the case of chloroform) or for a long period affecting several generations (example of mercury).

Lebailly et al. (2014) also proposed a dynamic freshwater ecotoxicity assessment for metals in LCA. After studying the behaviour of several metals, the authors reached the same conclusion as the present work: the integrated toxicity approaches the conventional value for large time spans, depending on the substance and compartment. However, in their method, the behaviour of non-persistent organic substances was not investigated. Concerning methodological aspects, their method is based on the time dependent calculation of CFs by solving Equation IV.3 for an initial unit load of substance (i.e. a pulse input, $g = 1\text{kg}$ at $t = \text{zero}$ and $g=0$ for $t>0$). CFs (instantaneous and cumulated) were calculated with a 1-year time step. Then, ecotoxicity impact (instantaneous and cumulated) was calculated at a given TH using the sum of the products $g(t)*CF(\text{TH}-t)$. The method proposed by Lebailly et al. (2014) differs from our method by the mathematical approach chosen for resolving the dynamic fate model.

Given that $g(t)$ is expected to be noisy with a complex shape representing the emission of a substance by many processes shifted in time, over a large time span covering the life cycle of a system, the most rigorous approach is to directly solve the ODE system, which was carried out in the present work.

The second solution could be to consider the mathematical properties of a linear system, i.e. the convolution product between an impulse response function of the system and the input perturbation signal. In our case, the system is the environment, the perturbation input signal is a substance entering the environment (a temporal emission $g(t)$), and the impulse response function IRF is the response of the environment (all environmental mechanisms taken together) at a pulse unit input ($g=\text{unit}$ at $t=0$, $g=0$ for $t>0$), i.e. a particular initial condition. This approach is similar to that of Lebailly et al. (2014): the $CFs(t)$ represent IRFs, and the toxicity calculation procedure they propose corresponds to a convolution product. Well before Lebailly et al, Hertwich (2001b) proposed, in a context different from LCA, to solve dynamic multimedia fate models by using the convolution approach, combined, in addition, with the Laplace transforms of equations and source function $g(t)$ in order to avoid numerical integration (possible only if $g(t)$ is analytically defined by a function).

The toxicity results obtained by the different mathematical methods presented (direct resolution of ODE and convolution approach) should be very similar, within the limit of inherent errors induced by the numerical resolution. However, given the behavioural complexity of the systems studied in the context of LCA, the convolution approach is more limiting while it requires specific mathematical conditions to be respected.

As regards the practicability of either of these approaches, again due to the complexity of the g function, the direct integration of dynamic mass balances is more practical and easier to handle in a

modelling platform where dynamic LCI and dynamic impact calculations are coupled (as described in paragraph 2.3 and shown in Figure IV.1). In addition, if the toxicity model should evolve by adding more dynamic phenomena, variable parameters in time and space, or spatial dimension, the direct resolution of a complex system of differential equations remains the only solution. Moreover, the calculation of time dependent CFs becomes unnecessary since the large number of values (many thousands for a single substance, depending on the granulometry of the time scale) make it unfeasible to use them in the spirit of conventional LCA (where only a single CF characterizes a substance/compartment pair). CF was a concept introduced in LCA for the sake of simplicity, in order to gather, in a single constant, the contributions of many environmental mechanisms and phenomena involved in the impact/damage generation. Thus in the dynamic context, characterization factors lose their sense and utility. This is why they are not used in the present study.

IV.3.2. Testbed case results

First of all, the “grape production” process was modelled in SimaPro[®] and the matrix of environmental interventions was extracted. The data from SimaPro[®] was then used in DyPLCA together with the necessary temporal parameters, resulting in a table containing 742 columns representing substances and compartments, with, in rows, the discrete values of environmental interventions (LCI) for each time step. The time span covered the lifetime of the main process (grape production, 25 years) and 1 year before for background processes (year⁻¹). The time step in the DyPLCA inventory used for this project was 0.5 days.

Then, data harmonization between the ecoinvent[®] and USEtox[®] databases was performed. Environmental compartments in ecoinvent are not defined in the same manner as in USEtox[®]. Thus, the adaptation of compartments led to a different number of combinations with the emitted substances (see SI IV.1 and 2 for more details). Moreover, the name and chemical speciation of substances are not the same in the ecoinvent and USEtox[®] databases, e.g. metals do not have an oxidation number in ecoinvent but they do in USEtox[®]. Speciation is one of the most important items of information for toxicity assessment. Finally, a total of 671 substance/compartment combinations were considered in this testbed case, covering emissions over the whole life cycle. The results obtained from DyPLCA, with harmonized nomenclature, were then used for dynamic toxicity calculation. The same harmonization was used for conventional LCI in order to calculate toxicity with steady-state USEtox[®].

For the sake of clarity, only the results for two selected substances are presented here together with results for organics and inorganics. All numerical results correspond to the functional unit, i.e. 1kg grape production. Figure IV.5.A presents the emission profile of one chosen substance, prochloraz, identified as one of the most impacting pesticide in this application, while Figure IV.5.B shows its

current mass (kg) in different compartments in function of time. The emission profile obtained after computing the dynamic LCI with DyPLCA tool, has peaks corresponding to the periods of application to the vines (see zoom side of the figure). These cycles can be well distinguished also on Figure IV.5.B as the pesticide is relatively rapidly degraded in agricultural soil and no major accumulation takes place from one cycle to another.

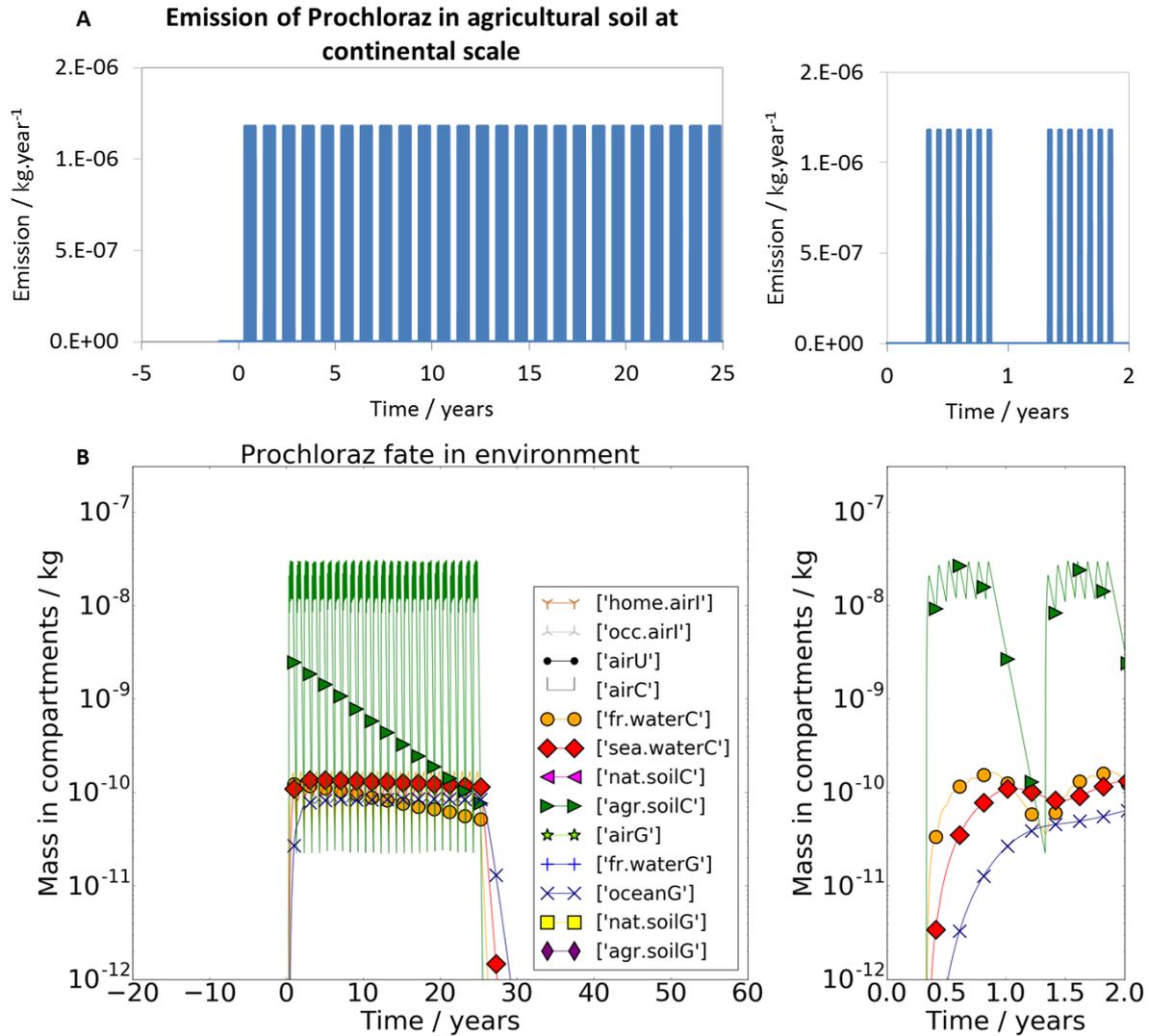


Figure IV.5 – Case of the prochloraz – results for 1kg grape production. (A): Emission into agricultural soil at continental scale with zoom between years 0 and 2. (B): Mass distribution in different compartments with zoom between years 0 and 2. Legend: home.airI = household indoor air, occ.airI = industrial indoor air, airU = urban air, airC = continental rural air, fr.waterC = continental freshwater, sea.waterC = continental sea water, nat.soilC = Continental natural soil, agr.soilC = Continental agricultural soil, airG = global air, fr.waterG = Global freshwater, oceanG = ocean, nat.soilG = Global natural soil, agr.soilG = Global agricultural soil.

It should be noted that emissions could occur in the life cycle of the process under study before it started to produce. For example, the production of grapes requires chemicals that are produced before the agricultural process. The start time of the grape production is noted $t=0$ but background processes had already been working before this time. Therefore, a negative part of the time axis was employed to point out the existence of background emissions in the past.

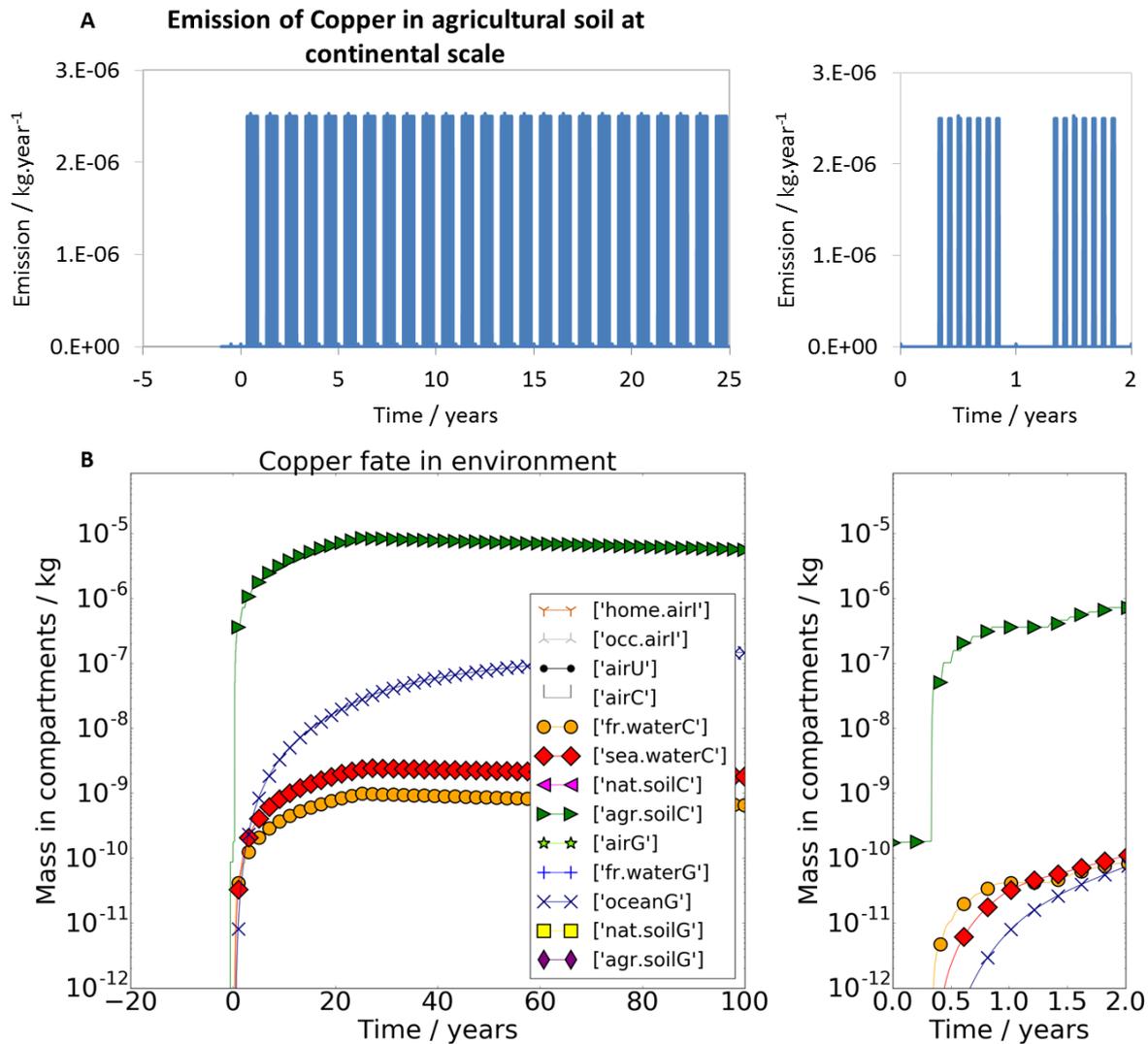


Figure IV.6 – Case of copper - results for 1kg grape production. (A): Emission profile into agricultural soil at continental scale with zoom between years 0 and 2. (B): Mass distribution in different compartments with zoom between years 0 and 2. Legend: home.airI = household indoor air, occ.airI = industrial indoor air, airU = urban air, airC = continental rural air, fr.waterC = continental freshwater, sea.waterC = continental sea water, nat.soilC = Continental natural soil, agr.soilC = Continental agricultural soil, airG = global air, fr.waterG = Global freshwater, oceanG = ocean, nat.soilG = Global natural soil, agr.soilG = Global agricultural soil.

Figure IV.6 shows the emission profile (A) and the fate (B) of copper, another compound present in pesticide products. The remaining mass is predominantly in agricultural soil at continental scale due to the slow transfer towards the other compartments and the very slow removal. The mass in this compartment increases until the last emission and then decreases slowly. About 64% of the mass still remains in the environment by the year 100 and 9% by the year 500.

The observed behaviours of the two substances shown similarities to those discussed in section 3.1, i.e. non-persistent organic compounds and persistent metals. Calculated dynamic toxicities follow the fate profile as discussed in section 3.1 (toxicity results presented in SI IV.7).

Figure IV.7 presents the results obtained for ecotoxicity in $\text{PAF}\cdot\text{m}^3\cdot\text{day}\cdot\text{day}^{-1}$ (Figure IV.7.A) and human toxicity, as cancer (Figure IV.7.B) and non-cancer (Figure IV.7.C) in $\text{cases}\cdot\text{day}^{-1}$, in function of time, for all substances emitted by the life cycle system. A highly variable toxicity profile is observed in the first 25 years (which is the lifetime of the foreground process), as a cumulated effect of organics and inorganics. After the end of emissions, the toxicity values drop to those of the remaining metals, and then decrease slowly following the fate of the metals.

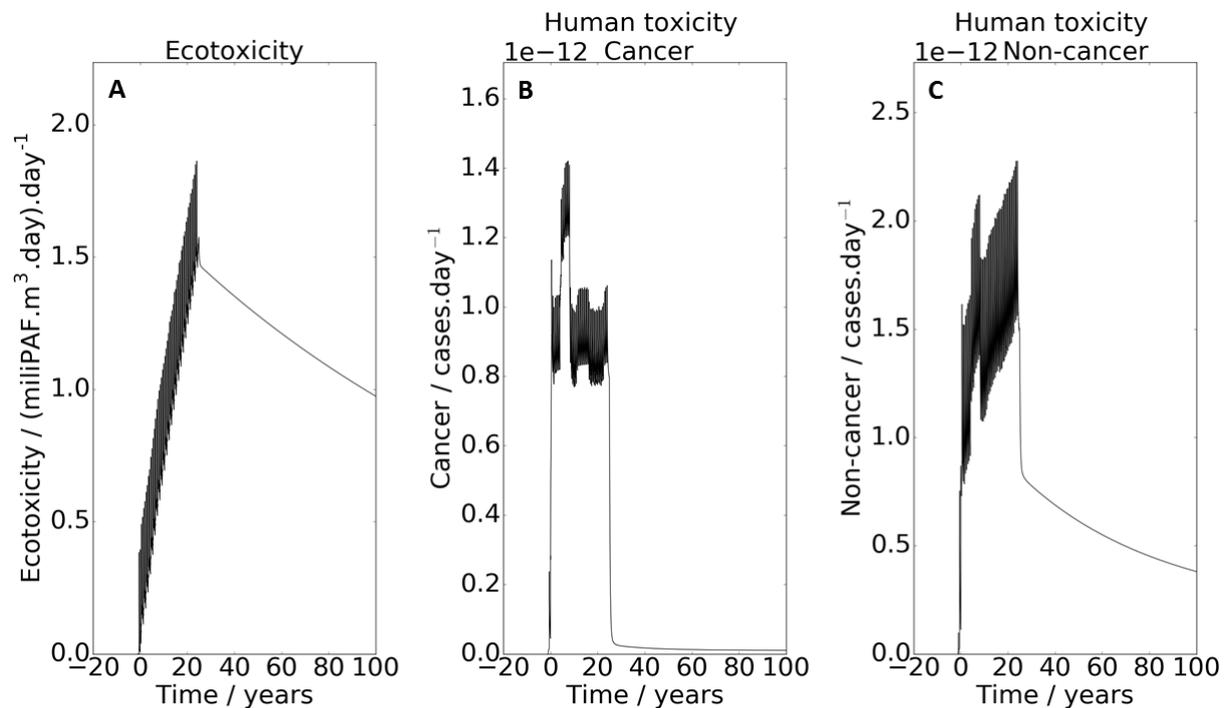


Figure IV.7 – Current toxicity for the production of 1 kg of grapes. (A) Ecotoxicity $n_{\text{eco}}(t)$; (B) Cancer and (C) Non-cancer Human toxicity $n_{\text{human}}(t)$.

Human toxicity and ecotoxicity were also calculated separately for organic and inorganic substances. Regarding the current ecotoxicity and human toxicity of organic substances (Figure IV.8 A, B and C), marked variations can be noted during the emission period as a result of the substance fate. As previously discussed and shown in the case of prochloraz, the fate of organic substances is driven not only by the emission profile but also by rapid removal and transfer processes. For the organic substances the impact is high during the emission period.

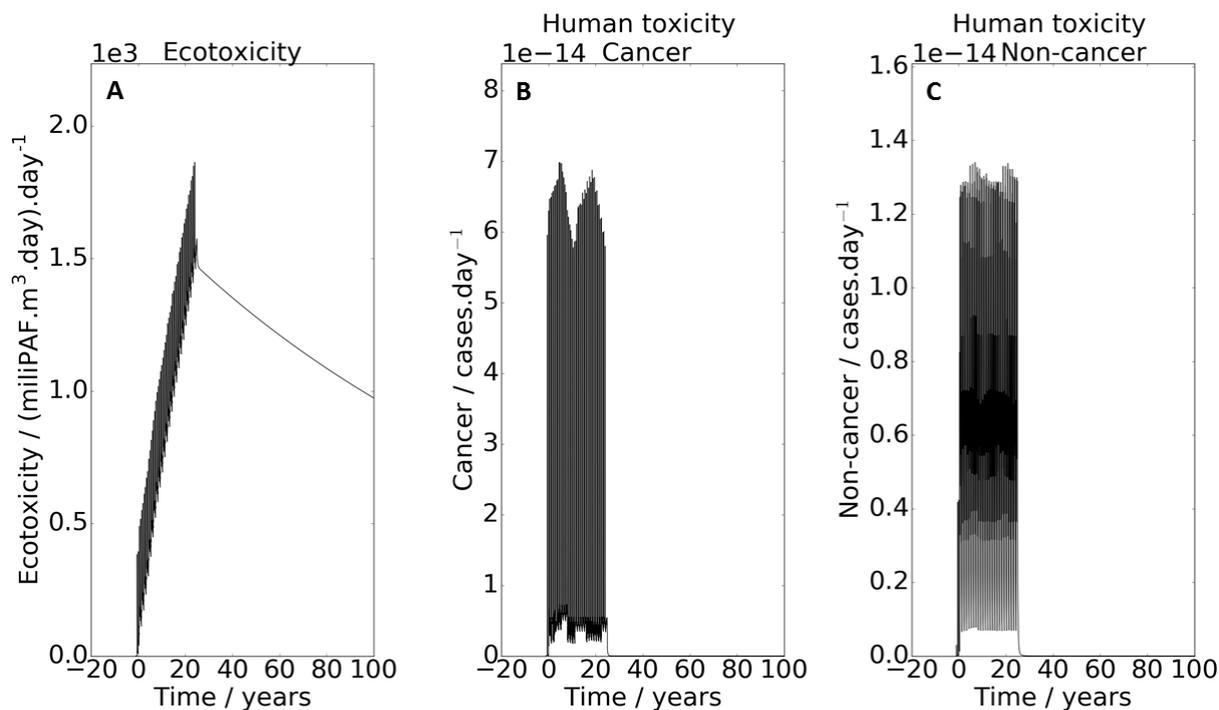


Figure IV.8 – Current Ecotoxicity $n_{eco}(t)$ (A), Cancer (B) and Non-cancer (C) Human toxicity $n_{human}(t)$ of organic substances for the production of 1 kg of grapes

Regarding the human toxicity and the ecotoxicity of inorganic substances (Figure IV.9 A, B and C), a large increase can be noted throughout the lifetime of the vineyard, due to the accumulation of substances in agricultural soil as a result of their slow inter-compartment transfer and very slow removal (high persistence). After that period, toxicities slowly decrease asymptotically in time.

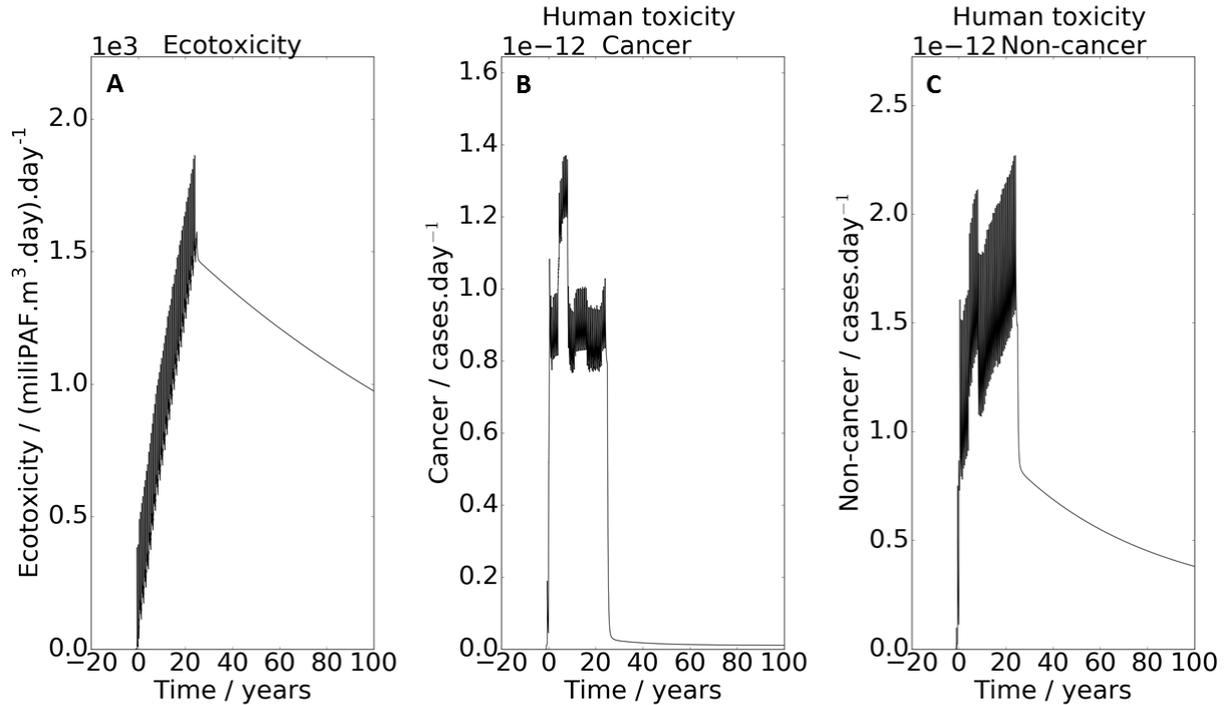


Figure IV.9 – Current Ecotoxicity $n_{eco}(t)$ (A), Cancer (B) and Non-cancer (C) Human toxicity $n_{human}(t)$ of metals for the production of 1 kg of grapes

Figure IV-10 shows the cumulated ecotoxicity in $\text{PAF}\cdot\text{m}^3\cdot\text{day}$ (Figure IV-10.A) and the cumulated human toxicity, as cancer and non-cancer in cases (Figure IV-10.B), over the time horizon, for all substances considered together, for organics and inorganics. Cumulated ecotoxicity and non-cancer human toxicity increased progressively with time due to the higher contribution of persistent inorganics. Cancer human toxicity increased strongly during the emission of pollutants and more slowly in the long term. The explanation is the contribution of less persistent inorganics with a high toxicity potential, such as arsenic or mercury (see SI IV.5).

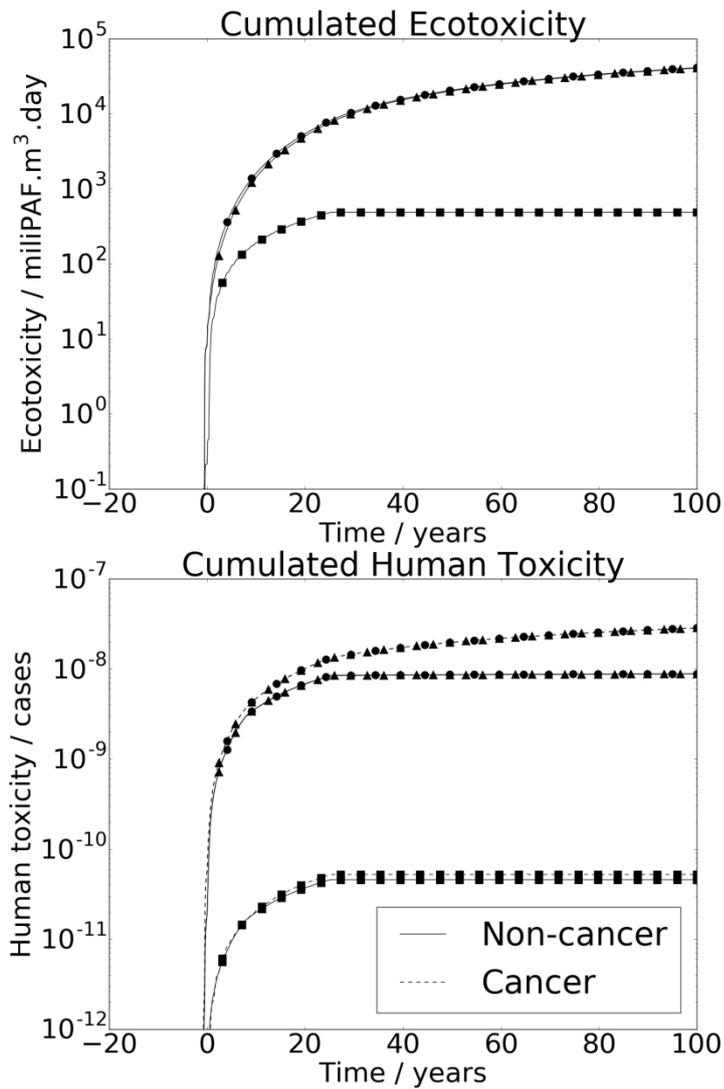


Figure IV-10 – Cumulated dynamic ecotoxicity $n_{eco,cumul}$ (A) and human toxicity $n_{human,cumul}$ (B) of all environmental interventions (●), organic substances (■) and metals (▲) for the production of 1 kg of grapes.

Cumulated toxicity for organic substances reflects their fate well. The order of magnitude of the cumulated values for toxicity of organic substances is negligible compared to the cumulated values of toxicity for all substances considered in the testbed case. Toxicity results for inorganic substances show values very close to those obtained for all substances which highlights the importance of inorganic substances in the toxicity impact assessment for this testbed case.

Table IV.3 presents the cumulated values for human toxicity and ecotoxicity, calculated over the time horizons of 100 and 500 years.

Table IV.3 –Conventional (infinite time horizon) and dynamic (time horizons of 100 and 500 years) cumulated toxicity impacts for organic, inorganic and all substances emitted in the grape production testbed case

	Cumulated impact	Conventional	Dynamic 100 years	Dynamic 500 years
Organic	Ecotoxicity (PAF.m ³ .day)	4.8E-01	4.8E-01	4.8E-01
	Cancer toxicity (cases)	5.7E-11	4.6E-11	4.6E-11
	Non-cancer toxicity (cases)	5.6E-11	5.2E-11	5.2E-11
Inorganic	Ecotoxicity (PAF.m ³ .day)	1.8E+02	4.1E+01	9.9E+01
	Cancer toxicity (cases)	1.2E-07	8.8E-09	1.0E-08
	Non-cancer toxicity (cases)	2.0E-07	2.8E-08	5.5E-08
All substances	Ecotoxicity (PAF.m ³ .day)	1.8E+02	4.1E+01	9.9E+01
	Cancer toxicity (cases)	1.2E-07	8.8E-09	1.0E-08
	Non-cancer toxicity (cases)	2.0E-07	2.9E-08	5.5E-08

When comparing the dynamic and conventional approaches for organic substances, a difference of about 20% can be observed in the case of human cancer toxicity. This difference may come from the inventory steps in conventional and dynamic LCI, which presented about 10% of difference. For metals, the gap between dynamic and conventional toxicity results decreases as the time horizon increases. In this work USEtox[®] was chosen as the database because it is highly recommended by LCA scholars. However, it should be noted that several data used for inorganic substances are of poor relevance (named interim values) and the results should be interpreted with caution.

When only the organic substances were evaluated, the following individual contribution results have been found (Table IV.4, more results in SI IV.7). The pesticide that had most influence for ecotoxicity was metam with a contribution of 32% in the dynamic and conventional methods; for dynamic human cancer toxicity, pronamide contributed with 12% in the dynamic method and 10% in the conventional method; for human non-cancer toxicity prochloraz contributed with 16% in the dynamic method and 15% in the conventional method.

Table IV.4 – Contribution of distinct pesticides on dynamic (cumulated toxicity at 100 years) and conventional (infinite time horizon) toxicity impacts generated by all organic substances. Results for human toxicity (Cancer and Non-cancer) and ecotoxicity (Eco) impacts for the production of 1 kg of grape.

Substance	Dynamic (100 years)			Conventional		
	Cancer	Non-cancer	Eco	Cancer	Non-cancer	Eco
Folpet	0.1%	0.2%	8.0%	0.1%	0.2%	8.1%
Thiram	0.0%	0.4%	1.9%	0.0%	0.4%	1.9%
Imidacloprid	0.0%	10.2%	0.7%	0.0%	9.3%	0.7%
Napropamide	0.0%	1.8%	0.1%	0.0%	1.7%	0.1%
Chlorothalonil	0.1%	2.5%	15.0%	0.1%	2.3%	15.2%
Pronamide	12.7%	4.7%	0.2%	10.2%	4.3%	0.2%
Pendimethalin	0.0%	4.7%	2.9%	0.0%	4.3%	2.9%
Metolachlor	0.0%	4.9%	3.7%	0.0%	4.5%	3.7%
Prochloraz	9.9%	16.1%	0.9%	7.7%	14.6%	0.9%
Mancozeb	0.0%	14.1%	14.4%	0.0%	13.0%	14.4%
Metiram	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
MCPB	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Glyphosate	0.0%	15.0%	1.0%	0.0%	0.0%	0.0%
Chlormequat	0.0%	11.4%	0.0%	0.0%	10.5%	0.0%
2,4-D	0.0%	9.0%	0.0%	0.0%	8.2%	0.0%
Metam-sodium dihydrate	0.0%	0.0%	31.7%	0.0%	0.0%	31.5%
Chlortoluron	0.0%	0.0%	0.3%	0.0%	0.0%	0.3%
Isoproturon	0.0%	0.0%	3.1%	0.0%	0.0%	3.1%
Metamitron	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Metazachlor	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Aclonifen	0.0%	0.0%	7.2%	0.0%	0.0%	7.2%
Dimethenamid	0.0%	0.0%	6.5%	0.0%	0.0%	6.5%

In this testbed case, cumulated toxicity and ecotoxicity are dominated by the inorganic persistent substances, for which conventional methods may give overestimated impact results, as also discussed in section IV.3.1. The more the TH tends to infinity the closer the value of cumulated toxicity comes

to the values of a conventional LCA. In contrast, current toxicity diminishes with TH. In other words, the population and ecosystems are less affected by the residual pollution but they suffer the greatest damage in a restricted period corresponding to the end of lifetime of the system (about one generation is strongly affected). These results emphasize the importance of the current impact evaluation as a measure of the intensity of possible damage at a given time.

Another aspect concerns the distribution in time of the activity of different processes involved in the life cycle of grape production. The dynamic LCI-LCIA approach allows observing that the main toxicity impact occurs in the present and future time. The explanation is that all chemicals and other commodities are produced and used during the lifetime of the foreground process and no important infrastructure was built in the past. The impact generated in the past by background processes, previously to vineyard activity, is very small when compared to the current impact (past impact is hardly visible on the negative time axis on all figures). However, inorganic substances emissions from the past activities generate persistent impact for the present and future time.

From a LCA – decision making point of view, dynamic evaluation provides complementary information helping at discriminating comparable scenarios and at proposing solutions for impact mitigation. For equal conventional impact results, time dependent behaviour of toxicity can be different for the compared scenarios. For example, scenario B has more metals contribution than A (all equal otherwise). Impact at the human lifetime scale could be lesser in case of B as the time horizon is a very important parameter for potential cumulated impact in case of persistent chemicals. Scenario B could be preferable for short durations like the vineyard lifetime. Solutions for changing the land destination could be envisioned in order to avoid a sensitive use (e.g. for food production) in the future.

The existence of variations with different amplitudes on the toxicity curves (Figures IV.5 and 9) suggests that dynamic toxicity simulation can be used as a forecast tool for, e.g. identifying optimal situations where certain activities should be (temporarily) stopped or, at the contrary, launched, at regional level. For example, to not use a specific substance during the years with forecasted high toxicity pics, or to stop the sensitive use of a certain water resource for a given period, etc.

IV.4. Conclusions

In this study, a mathematical implementation of dynamic toxicity assessment based on the USEtox[®] model was presented. In addition, the study developed a dynamic LCA framework, combining dynamic LCI modelling and toxicity impact evaluation over time. The feasibility of such an approach was demonstrated via a testbed case on grape production.

The main features of the dynamic toxicity calculator can be summarized as follows. The dynamic toxicity model is based on the resolution of the dynamic fate model in USEtox[®]. Exposure and effect factors are unchanged and considered constant in time. Characterization factors are no longer needed as current toxicity and cumulated toxicity are directly calculated in function of time.

Instead of using CFs, the dynamic mass balance equations were directly integrated, the behaviour of different substances being determined by the transport and reaction processes in the fate step. The computational method should consider the possibility of a noisy and random shape for the emission function. Therefore, the odeint integrator (Scipy Python), a robust method for ODE resolution that is compatible with stiff systems, was employed in the present work.

The toxicity calculator can be easily coupled with a dynamic LCI tool, in our case DyPLCA, thus providing a complete dynamic LCA framework.

Regarding the expected results of a dynamic approach, the following outcomes can be mentioned.

The current toxicity ($\text{cases}\cdot\text{day}^{-1}$) allows the intensity of the impact at a given time to be evaluated and the critical periods with regard to the potential impact to be identified. The evolution of toxicity in time is similar to the substance fate profile (mass in compartments versus time).

The cumulated toxicity (cases) represents the total damage generated over a given time horizon. This result was compared with the conventional toxicity value. It should be noted that the cumulated toxicity reaches the conventional toxicity value for large time horizons (theoretically at infinite time).

Significantly different behaviours were observed when persistent and non-persistent substances were compared. Non-persistent (generally organic) substances deployed almost all their hazard potential during their emission period and disappeared more or less rapidly due to degradation or transfer to sink compartments (removal). In contrast, persistent substances accumulated in environmental compartments during the emission period and their toxicity potential remained high after the cessation of emission, affecting many human generations. However, a calculation of toxicity at equilibrium (infinite time in conventional method) overestimated the total impact at the time scale of a human life.

The results obtained by the conventional method - which fixes an arbitrary time horizon - made no distinction between persistent and non-persistent pollutants. In contrast, dynamic calculations of toxicity and generally dynamic LCA brought out important information about the period when the potential hazard becomes critical, allowing mitigation of pollution issues, which is not the case in conventional LCA. Dynamic LCI – LCIA can be used as a forecast tool by simulating different scenarios in function of time, identifying optimal situations and scheduling the activities, helping in this way decision making. Combination of both dynamic aspects, LCI (share of environmental interventions in time, i.e. the functioning of life cycle processes) and LCIA (environmental mechanisms and specificities of substances), allows thus to obtain detailed case specific information on potential hazard/environmental impact.

Acknowledgements

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**Chapter V. Dynamic LCA:
Framework and sensitivity
analysis**

“The sensitivity of men to small matters, and their indifference to great ones, indicates a strange inversion.”

Blaise Pascal

The few studies related to the development of dynamic approaches in LCA focus on one specific step either LCI or LCIA (for only one impact category).

The objective of this chapter is to provide a complete framework for performing a dynamic LCA application including dynamics in LCI and LCIA steps. Methods, models and tools used for its development are explained as well the manner they were interconnected. Moreover, the temporal parameters needed for the calculation of the dynamic LCI and LCIA steps are presented. The framework is based in the methods and model which were already presented in the previous chapters (II, III and IV).

The choice of different values for the temporal parameters may lead to important differences in the results. The analysis of their influence in the dynamic method is then important in order to establish and interpret the outcomes of the dynamic model. Sensitivity analysis is a valuable tool to evaluate the relationship between the input and output variables of a system. Therefore, a sensitivity analysis was conducted on a case study (the life cycle of a waste water treatment plant). The choice of the case study was guided by the highly temporal variability of the physical parameters involved in that process, leading to a complex LCI temporal profile.

The presentation of the complete framework and the sensitivity analysis were submitted to the journal “Science of The Total Environment”.

For the case studies presented in the previous chapters, DyPLCA tool was not coupled with the temporal database as its development took a lot of time. The dynamic parameters for the background processes in the previous case studies were manually inputted which did not allow the exhaustive consideration of all background processes. Very recently a first version of the temporal database was finalized and implemented with DyPLCA tool. For this reason, a last case study (electricity mix scenarios from 2010 to 2090 in France) was performed in order to consider the connection of the whole dynamic framework with the temporal database.

Résumé

Les développements pour la prise en compte de la dimension temporelle dans l'ACV sont rares dans la littérature. De plus, les études réalisées à ce sujet se concentrent habituellement sur une étape spécifique de l'ACV. Beloin-Saint-Pierre et al. (2016) ont proposé une approche pour le calcul de l'inventaire dynamique et de l'impact changement climatique, et ils l'ont appliquée à un cas d'étude (la production d'eau chaude domestique). Cependant, ils ne considèrent que des valeurs agrégées pour l'évaluation dynamique de l'impact changement climatique. Aucune intégration avec une base de données pour la prise en compte du temps n'a été faite.

L'objectif de ce chapitre est de proposer une approche complète pour la réalisation d'une ACV dynamique, en prenant en compte l'aspect temporel dans les étapes d'ICV et EICV. La façon dont les modèles et les outils ont été interconnectés est expliquée, les paramètres temporels nécessaires au calcul des étapes d'ICV et EICV dynamiques sont présentés.

Le choix des valeurs pour les paramètres temporels peut entraîner des différences importantes sur les résultats finaux. L'analyse de leur influence dans la méthode dynamique est alors importante pour établir et interpréter le résultat du modèle dynamique. Par conséquent, une analyse de sensibilité a été effectuée sur un cas d'étude, à savoir le cycle de vie d'une usine de traitement des eaux usées. Le choix du cas d'étude a été guidé par la variabilité très importante des paramètres physiques impliqués dans ce processus, ce qui a conduit à un profil temporel d'ICV complexe.

La présentation de l'approche complète et l'analyse de sensibilité ont été proposées pour publication dans la revue *Science of The Total Environment*.

Dans les cas d'études présentés dans les chapitres précédents, l'outil d'ACV dynamique DyPLCA n'a pas été couplé avec la base de données temporelle. Les paramètres dynamiques pour les processus d'arrière-plan dans les études de cas précédentes ont été introduits manuellement, ce qui n'a pas permis la prise en considération de la plupart des procédés d'ecoinvent. La base de données temporelles a été finalisée dans sa première version à la fin du projet DyPLCA et donc de cette thèse. Pour cette raison, un cas d'étude a été réalisé à la fin de ce travail de thèse afin de considérer l'association de tous les outils avec la base de données temporelle.

En ce qui concerne l'analyse de sensibilité, comme remarque générale, les deux catégories d'impact présentent une grande variation par rapport à la période de calcul (100 ans dans cette étude), qui ne peut pas être captée dans une seule valeur d'impact pour un horizon de temps fixé. Au lieu de cela, une analyse détaillée est nécessaire au cours des premières décennies. La représentation graphique des résultats de l'ACV est très intéressante pour l'identification du profil temporel général.

Par conséquent, un horizon temporel fixé, tel qu'il est mis en œuvre dans les ACV conventionnelles, nous prive d'informations essentielles, en particulier pour les périodes courtes et moyennes correspondant à la durée de vie du système étudié et environ les vingt années suivantes.

Dans ce travail, il a été montré que les deux indicateurs dynamiques de réchauffement climatique ne sont pas sensibles à un pas de temps trop fin de définition de l'inventaire dynamique. Les simulations réalisées pour le même système, mais variant la granulométrie de l'ICV de 0.5 jour à 1 an, ont conduit à des résultats similaires. Le modèle de changement climatique dynamique n'est pas sensible non plus au changement du pas de temps pour la résolution numérique du modèle climatique. Pour l'étude de cas, un pas de temps de 1 mois a satisfait la condition de précision du résultat pour un effort de calcul très raisonnable.

Dans le cas de la toxicité, le niveau de détail de la définition de l'ICV (granulométrie temporelle) a une influence majeure sur les résultats. Dans les ACV classiques, l'état stationnaire est considéré pour la dispersion des substances dans l'environnement, c.-à-d. un horizon temporel infini. Ce travail a montré que la période la plus intéressante est celle pendant la durée de vie du système étudié et quelques décennies après.

Enfin, le cas d'étude a été porté sur le mix électrique français et son évolution pour les 60 années suivantes (jusqu'en 2080). Trois périodes sont distinguées, chacune d'une durée de 20 ans, pendant lesquelles les proportions des différentes sources d'électricité varient (réduction du % nucléaire et élimination des ressources fossiles). Cette étude a montré les capacités et les limites du cadre complet incluant l'ICV dynamique (plateforme web DyPLCA) avec intégration de la base de données temporelle et de l'EICV dynamique. La résolution du modèle dynamique a permis de retrouver 80% en moyenne de l'inventaire théorique pour tous les procédés et émissions. Les trois différentes périodes d'émission étaient bien distinguables et correspondaient au profil attendu, à l'exception de l'absence de paramètres temporels corrects pour les processus de traitement des déchets des infrastructures. De plus, la méthode d'EICV dynamique a montré que la méthode conventionnelle surestime généralement les résultats car les émissions sont toutes comptabilisées au temps zéro. La distribution des émissions dans le temps donne une perspective complètement différente des impacts.

Sensitivity analysis of temporal parameters in a dynamic LCA framework

Submitted as Shimako, A.H., Tiruta-Barna, L., Bisinella de Faria, A.B., Ahmadi, A., Spérandio, M. (2017). Sensitivity analysis of temporal parameters in a dynamic LCA framework (in preparation)

Abstract

Including the temporal dimension in the Life Cycle Assessment (LCA) method is a very recent research subject. A complete framework including dynamic Life Cycle Inventory (LCI) and dynamic Life Cycle Impact Assessment (LCIA) was proposed with the possibility to calculate temporal deployment of climate change and ecotoxicity/toxicity indicators. However, the influence of different temporal parameters involved in the new dynamic method was not still evaluated. In the new framework, LCI and LCIA results are obtained as discrete values in function of time (vectors and matrices). The objective of this study is to evaluate the influence of the temporal profile of the dynamic LCI and calculation time span (or time horizon in conventional LCA) on the final LCA results. Additionally, the influence of the time step used for the impact dynamic model resolution was analysed. The range of variation of the different time steps was from 0.5 day to 1 year. The graphical representation of the dynamic LCA results showed important features such as the period in time and the intensity of the worst or relevant impact values. The use of a fixed time horizon as in conventional LCA does not allow the proper consideration of essential information especially for time periods encompassing the life time of the studied system. Regarding the different time step sizes used for the dynamic LCI definition, they did not have important influence on the dynamic climate change results. At the contrary, the dynamic ecotoxicity and human toxicity impacts were strongly affected by this parameter. Similarly, the time step for impact dynamic model resolution had no influence on climate change calculation (step size up to 1 year was supported), while the toxicity model resolution requires adaptive time step definition with maximum size of 0.5 day.

Keywords: Dynamic Life Cycle Assessment, Sensitivity Analysis, Toxicity, Climate Change

V.1. Introduction

Life Cycle Assessment (LCA) is a widely used methodology for evaluating products and processes. LCA methodology consists of four operational steps: the definition of the goal and scope, the construction of the Life Cycle Inventory (LCI) based on mass and energy balances over the whole life cycle of the system, the Life Cycle Impact Assessment (LCIA) based on various impact calculation models, and the interpretation step (ISO, 2006a; ISO, 2006b). One of the recognized limitations of the LCA method is the lack of a time dimension in the definition of both the LCI and LCIA steps (Finnveden et al., 2009). Such a time dimension has only recently been integrated into LCA and little research is currently in progress.

Beloin-Saint-Pierre et al. (2014) have developed an approach called Enhanced Structure Path Analysis for considering time in the LCI step. Cherubini et al. (2011) have performed a calculation considering dynamic carbon removal by the biomass, which is a step leading up to the calculation of the climate change impact, while Levasseur et al. (2010) and Kendall (2012) have studied the time dependency of climate change impact by calculating temporal characterization factors (CF) for substances and applying them to dynamic emissions. Huijbregts et al. (2000a, 2000b, 2001), Hellweg et al. (2003) and Lebailly et al. (2014) have also proposed adjustments of conventional methods to include temporal characteristics in the toxicity category. In a recent study, Beloin-Saint-Pierre et al. (2016) proposed a complete framework for the calculation of a dynamic LCA. Tiruta-Barna et al. (2016) provided a dynamic method for LCI in which they took the complex supply chain and processes present in the LCA system into account. Their method can be linked to a conventional LCA database, which facilitates its use by LCA practitioners. Shimako et al. (2016, 2017) applied this dynamic LCI method in two different case studies, combining it with a dynamic climate change model and a dynamic toxicity model.

Numerous parameters can influence the temporal profile of a dynamic LCA result. At LCI level, these are physical parameters describing the process and supply chain dynamics, the time scale and its granulometry, and also specific parameters of the numerical methods used for model resolution. Dynamic LCIA results are determined by the choice of the impact models/submodels (i.e. static or dynamic) and their physical parameters, along with numerical method parameters.

The processes and phenomena involved in all these models are characterized by very different dynamics and thus prioritization of the most influent parameters is a necessity in the development of a dynamic LCA method.

Dyckhoff and Kasah (2014) analysed the influence of a time horizon in the calculation of the dynamic global warming potential indicator. A comparison between the cumulative and instantaneous

indicators demonstrated that contradictory conclusions could be drawn when different time horizons were used in calculations. The choice of a time horizon depends on the decision maker and is based more on policy than on scientific considerations. To the best of our knowledge, other important temporal parameters have not been analysed yet.

Sensitivity analysis is a valuable tool to evaluate the contribution of the temporal inputs to the dynamic results. There is general agreement that the input parameters of a model are sensitive in two distinct manners: (1) the uncertainty associated with an input parameter which is propagated in the model and contributes to the uncertainty of final results, or (2) the strong correlation between the inputs and outputs, such that a small change in the input leads to large changes in the output (Hamby, 1994). It is the second aspect that, at this stage of development of the dynamic approaches in LCA, allows the importance of the temporal parameters' influence on the LCA results to be identified, and will finally help further developments.

The objective of this work is to study the influence of temporal parameters involved in the dynamic LCA methodology we are currently developing. The global dynamic LCA framework was developed by using the dynamic inventory method proposed by Tiruta-Barna et al. (2016) and the dynamic impact assessment proposed by Shimako et al. (2016) and Shimako et al. (2017). One of the primary questions is how the dynamic LCI profile and the details of the inventory temporal definition will influence the final LCA results. In the aim of answering this question, a sensitivity analysis was conducted on a case study: a waste water treatment plant life cycle. The choice of the case was guided by the high temporal variability of the physical parameters involved in the process, leading to a complex LCI temporal profile.

V.2. Methods

V.2.1. Dynamic LCA framework

Global framework

The global framework for dynamic LCA is presented in Figure V.1.

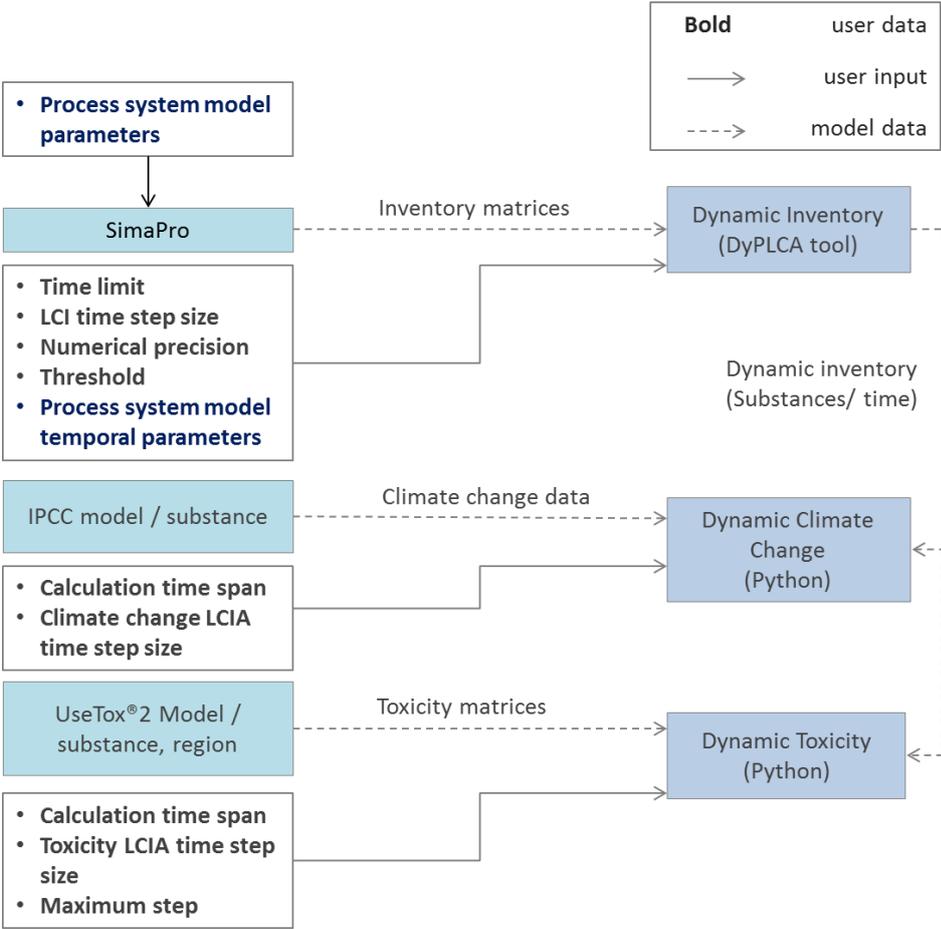


Figure V.1 – Parameters needed for the dynamic life cycle model in LCI and LCIA steps

First, SimaPro® LCA software was used for the traditional LCI resolution. This software delivers the LCI results in matrix form: a technological matrix and an environmental intervention matrix (interventions by compartments and processes). The dynamic inventory model and the DyPLCA software (web application <http://dypca.univ-lehavre.fr/>) start from the conventional inventory matrix to create the process flow network as a graph structure and then add temporal parameters related to processes and supply chains. After computation of the inventory model on the graph structure as a function of time, this tool delivers a time vector (days) and the associated environmental intervention vector (specific units.day⁻¹, e.g. kg. day⁻¹). Besides the temporal parameters specific to the processes and supply chains, the computation of a dynamic inventory requires specific parameters for the numerical methods (Figure V.1): time step size of graph resolution and consequently the time step size with which the LCI is calculated (e.g. values of inventory at each 0.5 day), backward time limit (the algorithm will stop when reaching a specific value of time backwards), numerical precision of the results and threshold (lower limit of the mass flow value that the algorithm will consider).

The result of the dynamic inventory, i.e. environmental interventions distributed in time, is used for the calculation of dynamic climate change and toxicity impact categories. Homemade Python programs were developed with this aim. For the calculation of dynamic impacts, data and phenomenological dynamic models were implemented: (i) from IPCC (IPCC, 2013) for climate change, and (ii) from the USEtox[®] 2 model (Hauschild et al. 2008; Rosebaum et al. 2008) for toxicity categories.

The parameters required for both climate change and toxicity, in addition to specific phenomenological parameters, are the time span for the impacts calculation and the time step size for the numerical calculation and for results retrieval. The maximum step for the ordinary differential equations (ODE) solver used to find the mass balance in the toxicity dynamic model must also be specified.

The principles of the dynamic models for climate change and toxicity impacts are briefly described below.

Dynamic climate change model

The dynamic climate change impact category was evaluated through two indicators: radiative forcing and global mean temperature change. The atmospheric burden, B_s , is an important parameter in the modelling of climate change potential. It can be calculated as the convolution product between the dynamic emission of the substance s , g_s ($\text{kg}\cdot\text{day}^{-1}$) and the impulse response function of that substance, IRF_s (Olivié and Peters, 2012) :

$$B_s(t) = \int_0^t g_s(t') \text{IRF}_s(t - t') dt' \quad \text{Equation V.1}$$

where t and t' are time scales. Radiative forcing is described as the product between the radiative efficiency, A_s , and the atmospheric burden, B_s . For sufficiently small emissions and approximately constant background conditions, the radiative efficiency A_s ($\text{W}\cdot\text{m}^{-2}\cdot\text{kg}^{-1}$) can be approximated as time-invariant (Joos et al., 2013). For emissions starting at time t_0 we have:

$$n_{\text{radiative forcing},s}(t) = \int_{t_0}^t A_s(t) g_s(t') \text{IRF}_s(t - t') dt' \quad \text{Equation V.2}$$

The dynamic global warming potential ($n_{\text{radiative forcing}}(t)$ in $\text{W}\cdot\text{m}^{-2}$) for all gases taken together is then:

$$n_{\text{radiative forcing}}(t) = \sum_s n_{\text{radiative forcing},s}(t) \quad \text{Equation V.3}$$

Then, the global warming potential for all gases ($n_{\text{radiative forcing}}$ in $\text{W}\cdot\text{m}^{-2}\cdot\text{day}$) over a given time span TH is:

$$n_{\text{radiative forcing}} = \int_{t=t_0}^{TH} n_{\text{radiative forcing}}(t) dt \quad \text{Equation V.4}$$

The second indicator, i.e. global temperature potential, is defined as the convolution product between the radiative forcing and the temperature impulse response function (Olivié and Peters, 2012):

$$n_{\text{temperature},s}(t) = \int_{t_0}^t \left(\int_{t_0}^t A_s(t) g_s(t') \text{IRF}_s(t-t') dt' \right) \text{IRF}_T(t-t') dt' \quad \text{Equation V.5}$$

where $n_{\text{temperature},s}(t)$ is the global temperature potential for a substance s at time t and IRF_T is the temperature impulse response function, which is independent of the type of GHG. The mean temperature change at a given time t , $n_{\text{temperature}}(t)$ (K), is obtained by aggregating values for all the substances concerned:

$$n_{\text{temperature}}(t) = \sum_s n_{\text{temperature},s}(t) \quad \text{Equation V.6}$$

Dynamic toxicity model

The dynamic toxicity approach was developed in Shimako et al. (2017) and only a brief background is presented below. Traditionally, toxicity impact is calculated as the product of the substance mass and its characterization factor (CF). CF is the result of combined models for substance fate in environment (fate factor), exposure of organisms to the hazardous substance (exposure factor) and the negative effects of the substance (effect factor). The dynamic approach replaces the fate factor by a dynamic model of substance fate while keeping the exposure and effect factors from the conventional approach. The fate model of a substance in the environment considers distinct mechanisms, such as the transport between compartments, reaction processes (e.g. degradation), and removal (immobilization in

different media). The mass balance of a substance in the environment is described by a system of ODE (Mackay, 2002):

$$\frac{dm_s}{dt} = K_s m_s + g_s \quad \text{Equation V.7}$$

where K is the square matrix of rate constants (related to removal, degradation and transport processes) in each compartment i (day^{-1}), m is the mass vector of substance s in the respective environmental compartments (kg), g is the vector of emission flows in each compartment (kg day^{-1}), and t is time.

The generic dynamic fate model was adapted with the USEtox[®] toxicity model (specific parameters per substance and phenomenon, 13 environmental compartments; Joliet et al., 2006; Ligthart et al., 2004; McKone et al., 2006). By the end of the calculation, a mass vector (13 values corresponding to each compartment) had been obtained for each discrete time value. For the toxicity results, following the matrix approach proposed by Rosenbaum et al. (2007), each mass vector is multiplied by the exposure matrix (XF) and effect matrix (EF):

$$n_{human,s}(t) = m_s(t) \times XF_{human,s} \times EF_{human,s} \quad \text{Equation V.8}$$

$n_{human,s}(t)$ is the vector that represents human toxicity (cancer and non-cancer, cases.day^{-1}) for a certain substance s in different compartments, at a given time t .

$$n_{eco,s}(t) = m_s(t) \times XF_{eco,s} \times EF_{human,s} \quad \text{Equation V.9}$$

$n_{eco,s}(t)$ represents the ecotoxicity expressed in $(\text{PAF.m}^3.\text{day}).\text{day}^{-1}$, due to an emission into a specific compartment for a certain substance s at a given time t .

The result for the aggregation of all substances s and compartments i , for a given time t , is obtained by:

$$n_{human}(t) = \sum_s \sum_i n_{human,s,i}(t) \quad \text{Equation V.10}$$

$$n_{eco}(t) = \sum_s \sum_i n_{eco,s,i}(t) \quad \text{Equation V.11}$$

The cumulated values, $n_{human,cumul}$ (cases) and $n_{eco,cumul}$ (PAF.m³.day) for human toxicity and ecotoxicity can then be calculated:

$$n_{human,cumul}(TH) = \int_{t=t_0}^{TH} n_{human}(t) \quad \text{Equation V.12}$$

$$n_{eco,cumul}(TH) = \int_{t=t_0}^{TH} n_{eco}(t) \quad \text{Equation V.13}$$

where t_0 represents the time of the first emission into the environment and TH is the time span for which the cumulated impact is calculated.

It is worth noting that both dynamic approaches, climate change and toxicity, provide impact results at any point in time and are independent of the notion of time horizon – a key and controversial concept in conventional LCA.

V.3. Case study

In this work, a conventional wastewater treatment plant, WWTP, was used for a case study. The reason for this choice was the high variability of treatment conditions, leading to variable environmental interventions in time. The case study allowed a detailed analysis of the influence of temporal parameters on the dynamic impact results.

Goal and scope definition

A conventional and a dynamic LCA were performed and the results were compared for the target impact categories: climate change, human toxicity and ecotoxicity. Determining the sensitivity of the LCA results to temporal parameters was the main objective of this work.

The unit function was 1 m³ of waste water treated respecting the regulatory rejection limits for the outlet effluent (water discarded into the environment) and the plant lifetime was taken as 30 years.

LCI

Figure V.2 shows the flowsheet of the WWTP studied. It comprised a primary clarification unit, 2 anoxic tanks and 3 aerobic tanks. A post denitrification zone was also added to achieve acceptable effluent quality. Nitrate was recycled from the aerobic to the anoxic zone. The sludge was separated in a secondary clarifier, which was also partly a wastage flow redirected to a thickener, and partly recycled in the anoxic zone. The resulting sludge was sent to incineration and the effluent discarded into the environment.

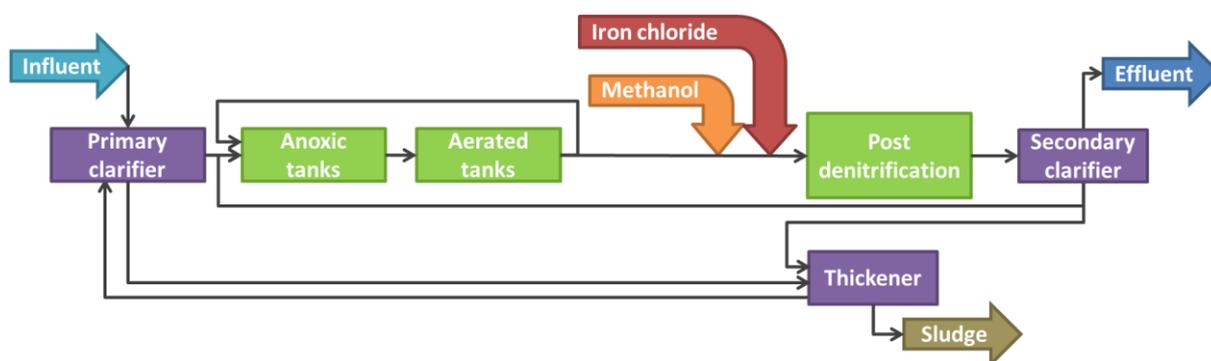


Figure V.2 – Schema of the WWTP considered in the case study

WWTP unit processes involve a large number of biological and chemical reactions with various dynamics. Modelling all the processes would be extensive and time consuming. For this reason, the dynamic simulation of the WWTP (the foreground process in LCA) was performed in Sumo[®] software, a wastewater treatment process simulator that includes biological, chemical, and physical processes. The database ecoinvent 3.2 was used for the background processes such as the production of raw materials, energy and infrastructure.

External carbon (methanol) was required to complete the denitrification, and iron chloride (FeCl₃) was added to chemically precipitate phosphorus in the sludge. Both additions were also necessary in order to satisfy legal discharge requirements for the effluent. The use of methanol releases carbon dioxide (CO₂), a percentage of which originates from a fossil source and should be taken into account in the inventory. Emissions of N₂O from WWTPs are considered to be 0.5% of nitrified ammonia flows in dynamic conditions (Czepiel et al., 1995). The volume and composition of off-gas were calculated (in Sumo[®] software) using gas/liquid transfer models. Calculations were based on transfer coefficients and concentration gradients with the atmosphere.

Heavy metal concentrations are not taken into account by Sumo[®] as these metals are considered to be inert for biological processes. Their input concentrations in WWTPs were therefore taken from Doka (2009) and Henze and Ledin (2001) and allocated to effluent and sludge in specific quantities, using the specific transfer coefficients proposed by the same authors.

The electricity consumption was calculated by taking the sum of all requirements: aeration of aerobic and nitrification tanks and thickener, mechanical mixing of anoxic tanks, pumping of main lines (influent input, dosing of chemicals, sludge output, recirculation lines, and effluent output), scraping and dewatering unit. Incineration of the sludge took account of gas-emissions in the form of CO₂, and metals (copper, lead and zinc).

WWTP basic infrastructure was included using a class 2 capacity data set from ecoinvent (which includes dismantling) and an annual sewage volume of approximately 1.4E7 m³ was considered.

All inventory results are presented in SI V, along with the ecoinvent reference for each flow.

Dynamic LCI

The flow rate and composition of the influent to a WWTP is commonly subject to time variations, i.e. low rate during the night and high rate during the day, weekend effect, influence of holidays, and seasonal effects (Gernaey et al., 2011) (flow variations presented in SI V). In order to include these variations in the plant dynamic model, the influent generator of Gernaey et al. (2011) was used. Thus, it was considered that the operation of the plant and the influent it received had variable and cyclic behaviour with a period of 1 year. Consequently, the inventories of the foreground processes (direct emissions of CO₂, CH₄ and N₂O by the plant; CO₂, N₂O, heavy metals and organic substances from sludge treatment) and of the supply chain (iron chloride, methanol and electricity consumption) were also variable. The variations of emissions in the WWTP were calculated with Sumo[®] for the interval of one year and the results were replicated for every year of its life span.

Raw materials (methanol, iron chloride) were considered to be supplied every 2 months (delay of 60 days and production period of 1 day). Electricity was considered to be supplied continuously during the life time of the WWTP. The time considered for the infrastructure construction of the WWTP was 3 years for the processes of building and 6 months' delay for the plant start up. The temporal parameters used for the background processes are shown in SI V. The temporal behaviour of the background environmental interventions was calculated with the web-tool DyPLCA (Tiruta-Barna et al., 2016).

The inventory results obtained with Sumo and DyPLCA are in the form of discrete values in time for a predefined time step of 0.5 days. This time step corresponds to the smallest duration for a significant variation of physical parameters involved in the WWTP operation (variation of the influent flow rate

for instance). Coarser time granulometries can also be used, for capturing daily, monthly or seasonal variations. Consequently, additional time step sizes were analysed: 1 day, 1 week, 1 month, 1 season and 1 year. The discrete values of the initial dynamic inventory were thus recalculated for each time granulometry:

$$g_s(t)_{\Delta t_{higher}} = \frac{1}{\Delta t_{higher}} \sum_{t'=n}^{n+m-1} g_s(t')_{\Delta t_{lower}} \Delta t_{lower} \quad \text{Equation V.14}$$

for $n = (t_0, t_0 + m, t_0 + 2m, \dots, t_{final})$ and $m = \frac{\Delta t_{higher}}{\Delta t_{lower}}$

where t is the discrete time value for the new time scale granulometry; t' is the discrete time value in the initial LCI time scale (step size of 0.5 days); s is the substance being analysed, t_{final} is the discrete time at which the last emission of the dynamic inventory is released (day); $g_s(t')$ is the mass flow value for a specific substance and for a specific time t' , which is the result of the dynamic LCI ($\text{kg}\cdot\text{day}^{-1}$), Δt_{lower} is the time step used for the calculation of the dynamic LCI (i.e. 0.5 days), Δt_{higher} is the new time step required and t_0 is the initial time in the dynamic LCI.

In this way, the same total quantity of a substance can be differently distributed in time (with different granulometries), leading to different profiles of the dynamic LCI, $g_s(t)$.

Conventional LCI values, $g_{s,total}$ (kg), can be retrieved by the time integration of the dynamic LCI:

$$g_{s,total} = \int_{t=t_0}^{t_{final}} g_s(t) dt \quad \text{Equation V.15}$$

LCIA

The impact categories chosen in this study are those for which a dynamic approach exists, as presented in section 2.1. The IPCC climate change and USEtox[®] toxicity models are the basis of the dynamic impact models and were also used in conventional LCA applied to the case under study.

A calculation time span of 100 years was chosen for both dynamic impacts. In conventional LCA, a time horizon of 100 years is commonly used for climate change while, for toxicity categories, an infinite time horizon is considered.

V.3.1. Sensitivity analysis

Dynamic inventory results represent the emission variations due to the behaviour of the supply chain and processes. Moreover, dynamic impact assessment is based on environmental models that can be sensitive to different time scales (days, months, years, decades, etc.). One of the major questions subsequent to a time dependent approach of LCA concerns the extent to which the temporal parameters influence the LCA results and, in particular, how the time granulometry used in the definition of the dynamic flows will affect the temporal profile of the calculated impacts.

To investigate this, the influence of each of the following parameters was analysed: i) the detail of the temporal definition of the inventory (a process and supply chain characteristic), ii) the calculation time span (time horizon in conventional LCA) for the dynamic impact methods, iii) the time step size resolution of the dynamic impact models (including the ODE specifications).

For this study, several emissions from the system's life cycle were selected based on a significant variation in their temporal profile, and also based on their important contribution to the LCA results as pointed out by previous studies (Bisinella de Faria et al., 2015; Bisinella de Faria et al., 2016). In this sense, CO₂, CH₄ and N₂O were considered as they are direct emissions from the WWTP, from sludge incineration and from the infrastructure processes. Metals emitted by sludge incineration (copper, zinc, lead, chromium, mercury) and infrastructure processes (mercury) were analysed, all of them being included in the USEtox[®] database. Phenomenological parameters inherent to the LCIA models had already been investigated for climate change and toxicity in other studies (IPCC, 2013; Henderson et al. 2011; Rosebaum et al. 2011) and were not analysed in this work.

Several approaches exist for sensitivity analysis, such as variance decompositions, partial derivatives or elementary effects. A one-at-a-time sensitivity method was used, i.e. the effects of only one parameter were investigated at a time. The sensitivity indicator is the relative difference between the impact results of a given scenario (with a modified parameter) and the reference scenario (reference values for the temporal parameters), calculated by:

$$\text{relative difference (t)} = \frac{n(t)_{\text{step}} - n(t)_{\text{step}}^{\text{ref}}}{n(t)_{\text{step}}^{\text{ref}}} \quad \text{Equation V.16}$$

where $n(t)_{\text{step}}$ is the impact value at time t for the calculation scenario with a variable temporal parameter 'step' (e.g. LCI time step size), 'ref' indicates the reference calculation scenario with predefined values for the temporal parameters (e.g. LCI time step of 1 year).

V.4. Results and discussion

V.4.1. Influence of the dynamic LCI profile and the time span of the impact calculation

Figure V.3 shows the dynamic LCI results for the emission of carbon dioxide in kg.day⁻¹ during the life cycle of the WWTP studied. The different graphics of Figure V.3 were obtained for LCI time step sizes of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

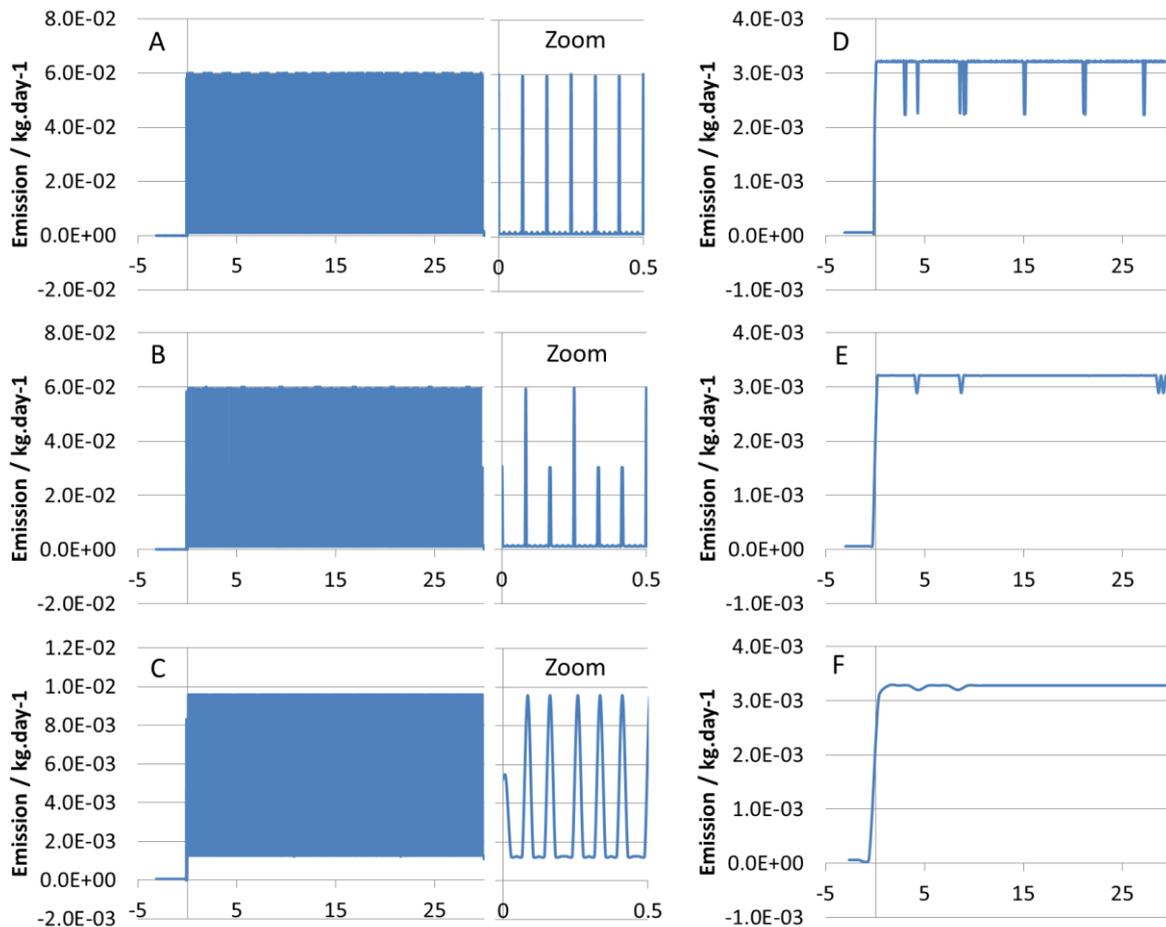


Figure V.3 – CO₂ emission by the life cycle system of a WWTP. Dynamic inventory for different time step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, E- 1 season and F- 1 year). Zoom on the year between 0 and 0.5 for A, B and C.

Figure V.3.A, B and C show the important influence of the variation of emissions due to the different temporal characteristics of the process. On the other hand, the profile of emissions represented in the Figure V.3.D, E and F tend to a constant value around 3.3E-3 kg.day⁻¹, representing almost steady state conditions. For this reason, the calculation scenario with the time step of 1 year was chosen as the reference calculation scenario (ref in formula 16). The maximum time step for which the inventory

variations can be clearly distinguished is a week for this case study. The amplitude of the emissions also change: the values for the emissions in Figure V.3.A range between 0 and 0.06 kg.day⁻¹ while they range only between 0.001 and 0.01 kg.day⁻¹ in Figure 3.C.

LCI results for different time steps are available for all the substances selected in this work. The mass balance was verified by calculating the cumulated inventory $g_{s,total}$ per substance. Table V.1 shows that the values do not present any great variation when the step size is changed. The calculation of the relative difference between the cumulated values for different step sizes and the reference (time step size of 1 year) did not exceed 1%. These results are in accordance with the mass balance, which does not change with the calculation time step.

Table V.1 – Cumulated LCI results for WWTP case study calculated with different time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year).

	Carbon dioxide	Methane	Dinitrogen monoxide	Copper	Lead	Zinc	Copper
0.5 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 day	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 week	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 month	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 season	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.1E-08
1 year	9.5E-02	2.1E-04	2.9E-06	2.0E-06	1.9E-06	1.1E-05	2.0E-08
	Lead	Zinc	Methylene chloride	Chloroform	Chromium III	Mercury	
0.5 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 day	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 week	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 month	2.0E-08	1.1E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 season	2.0E-08	1.2E-07	7.9E-08	1.7E-07	3.3E-09	2.9E-11	
1 year	2.0E-08	1.1E-07	7.8E-08	1.7E-07	3.3E-09	2.9E-11	

Climate change results

Figure V.4 shows the comparison between the results for dynamic mean temperature change and cumulated radiative forcing, calculated with different inventory step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year) for a time span of 100 years. Carbon dioxide, methane and dinitrogen monoxide were considered. The step size used for the calculation of the dynamic climate change impact was 0.5 days.

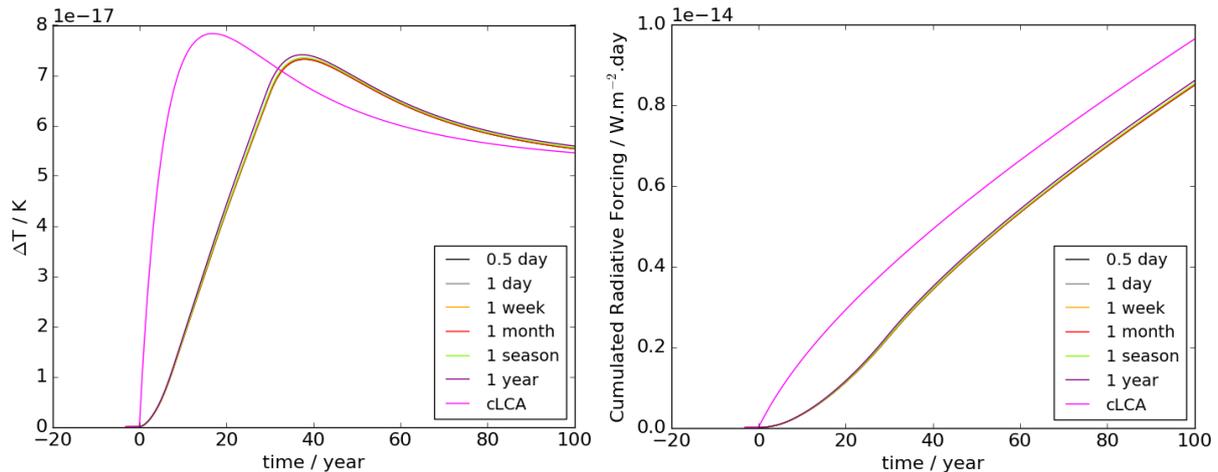


Figure V.4 – Mean temperature change and cumulated radiative forcing for the case study of the WWTP, calculated for a time span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year. Results for conventional methods: cLCA curve.

No noteworthy difference could be seen between the curves corresponding to the dynamic method, highlighting the low response of the climate change model (both indicators) to the temporal variations of emissions at daily to monthly levels.

Table V.2 details the relative difference between the values calculated with the dynamic model for different LCI time step sizes and the case when step size was 1 year. The case of step size of 1 year is considered as the reference since the plant behaves as steady state system with constant emissions. The values of dynamic impact for both climate change indicators were calculated at year 100. At this time point, they did show a marked difference when the LCI step size was modified.

As expected, the lower the time step size, the higher the relative difference (with respect to the steady state emission) in the climate change results. However, these results show that the dynamic model is not significantly sensitive to the time step size of LCI (at least for the present case study and similar systems) at any time. This allows a higher time step size to be used in the dynamic inventory calculation, which is more practical and easier to obtain, and requires less computational work and time.

Regarding the conventional mean temperature change in Figure V.4 (left side), this method considers that the emission occurs at time 0. The maximum value for mean temperature change is higher for the conventional method than for the dynamic method. The conventional method gives a maximum value of $7.8E-17$ K and it is reached by year 16. For the dynamic method, the maximum value is $7.4E-17$ K by year 37. The result obtained at year 100 is similar for both methods, presenting a value of around $5.5E-17$ K. The cumulated radiative forcing is the impact indicator in the conventional climate change

impact method. In Figure V.4 (right), the values attained at year 100 are around $8.5E-15 \text{ W.m}^{-2}.\text{day}$ for the dynamic method and $9.6E-15 \text{ W.m}^{-2}.\text{day}$ for the conventional method. The difference between dynamic and conventional results is almost constant during the whole calculation period, showing that the conventional calculation overestimates the impact from the beginning.

Table V.2 – Relative difference of mean temperature change and cumulated radiative forcing for a time span of 100 years. The reference is the case of LCI time step size of 1 year. LCI time step sizes of 0.5 day, 1 day, 1 week, 1 month and 1 season were analysed.

Relative difference of ΔT results at year 100 (K)					
Substance	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	-1.2%	-1.2%	-1.2%	-1.1%	-0.8%
Methane	-0.6%	-0.6%	-0.5%	-0.4%	-0.3%
Dinitrogen monoxide	-1.1%	-1.1%	-1.1%	-1.0%	-0.8%
All substances	-1.2%	-1.2%	-1.2%	-1.1%	-0.8%
Relative difference of cumulated radiative forcing results at 100 years ($\text{W.m}^{-2}.\text{day}$)					
Substance	0.5 day	1 day	1 week	1 month	1 season
Carbon dioxide	-1.6%	-1.6%	-1.5%	-1.4%	-1.1%
Methane	-1.2%	-1.2%	-1.1%	-1.0%	-0.8%
Dinitrogen monoxide	-1.5%	-1.6%	-1.5%	-1.5%	-1.1%
All substances	-1.3%	-1.3%	-1.3%	-1.3%	-0.9%

Table V.3 shows the mean temperature change and cumulated radiative forcing values for the WWTP case study at a time span of 100 years. It also shows the relative difference between dynamic and conventional values in parentheses. Considering the mean temperature change for a time span (or time horizon) of 100 years, methane presented a large difference, of about 20%, between the conventional and dynamic results. On the other hand, the relative difference between the conventional and dynamic mean temperature change values for carbon dioxide was quite small, about 3%.

Considering the comparison between the dynamic and conventional cumulative radiative forcing, there is almost no difference for the methane results. On the other hand, dinitrogen monoxide and carbon dioxide present large differences. The global cumulated radiative forcing is higher in conventional LCA than in the dynamic approach, which signifies that, for a time horizon of 100 years, conventional LCA overestimates the climate change impact.

Table V.3 – Dynamic and conventional climate change (cLCA) values (mean temperature change and cumulated radiative forcing) for a time span of 100 years. In parentheses are the relative differences between conventional and dynamic values.

Mean ΔT value at year 100 (K)							
Substance	Dynamic inventory step size						cLCA
	0.5 day	1 day	1 week	1 month	1 season	1 year	
Carbon dioxide	5.3E-17 (2.3%)	5.3E-17 (2.3%)	5.3E-17 (2.4%)	5.4E-17 (2.5%)	5.4E-17 (2.8%)	5.4E-17 (3.6%)	5.2E-17
Methane	5.7E-19 (19.3%)	5.7E-19 (19.3%)	5.7E-19 (19.4%)	5.7E-19 (19.6%)	5.7E-19 (19.6%)	5.8E-19 (20.0%)	4.8E-19
Dinitrogen monoxide	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.3%)	4.1E-19 (9.4%)	4.1E-19 (9.7%)	4.1E-19 (10.5%)	3.7E-19
All substances	5.4E-17 (2.5%)	5.4E-17 (2.5%)	5.4E-17 (2.6%)	5.4E-17 (2.7%)	5.5E-17 (3.0%)	5.5E-17 (3.8%)	5.3E-17
Cumulated radiative forcing at 100 years ($W \cdot m^{-2} \cdot day$)							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Carbon dioxide	7.7E-15 (-12.0%)	7.7E-15 (-12.0%)	7.7E-15 (-12.0%)	7.7E-15 (-11.9%)	7.7E-15 (-11.6%)	7.8E-15 (-10.6%)	8.8E-15
Methane	5.3E-16 (-0.6%)	5.3E-16 (-0.6%)	5.3E-16 (-0.5%)	5.3E-16 (-0.4%)	5.3E-16 (-0.2%)	5.4E-16 (-0.6%)	5.4E-16
Dinitrogen monoxide	6.3E-17 (-10.8%)	6.3E-17 (-10.9%)	6.3E-17 (-10.8%)	6.4E-17 (-10.7%)	6.4E-17 (-10.5%)	6.4E-17 (-9.4%)	7.1E-17
All substances	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-9.3%)	8.5E-15 (-8.9%)	8.6E-15 (-8.1%)	9.4E-15

Table V.3 also points out that the values obtained for all substances taken together are very close to the values obtained for CO₂, which is explained by the fact that CO₂ is the major GHG in this case study. Obviously this behaviour cannot be generalized.

In order to flesh out the results observed above, Figure V.5 shows the results obtained for methane with the same calculation conditions as for Figure V.4. Here too, no important difference can be seen between the curves obtained for various inventory time step sizes. The maximum value for mean temperature change is higher for the conventional method than for the dynamic method. It has a value of 1.2E-17 K, which is reached by year 10. For the dynamic method, the maximum value is 9.5E-18 K by year 30. Both curves tend towards a low limit as methane has a limited lifetime in the atmosphere and is transformed into CO₂.

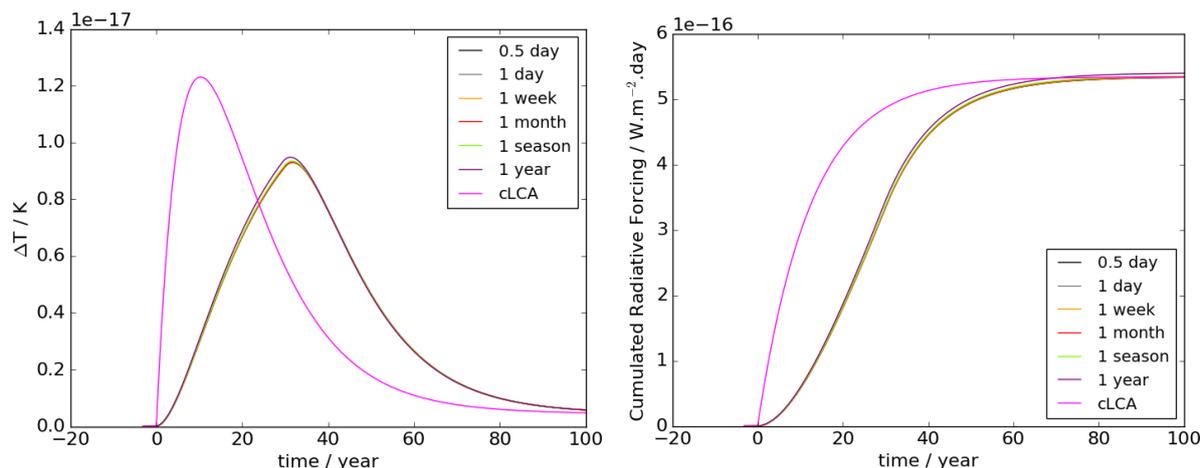


Figure V.5 – Mean temperature change and cumulated radiative forcing for methane calculated for a time span of 100 years. Dynamic LCI inventory step sizes analysed: 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year. Results for conventional method: cLCA curve.

Figure V.4 and Figure V.5 clearly show that the effects in terms of mean temperature change and cumulated radiative forcing have amplitudes and positions on the time scale that depend on the GHG emission duration and time position, and on the lifetime of each GHG. In conventional LCA, all information related to the time occurrence of the (worst) effects, at the human time scale of about 100 years, is lost by the zero time point emission on one hand, and by an arbitrarily chosen time horizon on the other. For industrial processes with lifetimes of about 20 – 30 years, a time horizon of 100 years (or any other fixed value) is not suitable. Instead, dynamic methods offer the possibility of monitoring the climate change indicators over time.

Toxicity

Figure V.6 shows the dynamic LCI results for the emission of chloroform in kg.day⁻¹ during the life cycle of the WWTP studied. The different graphics of Figure V.6 were obtained for step sizes of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

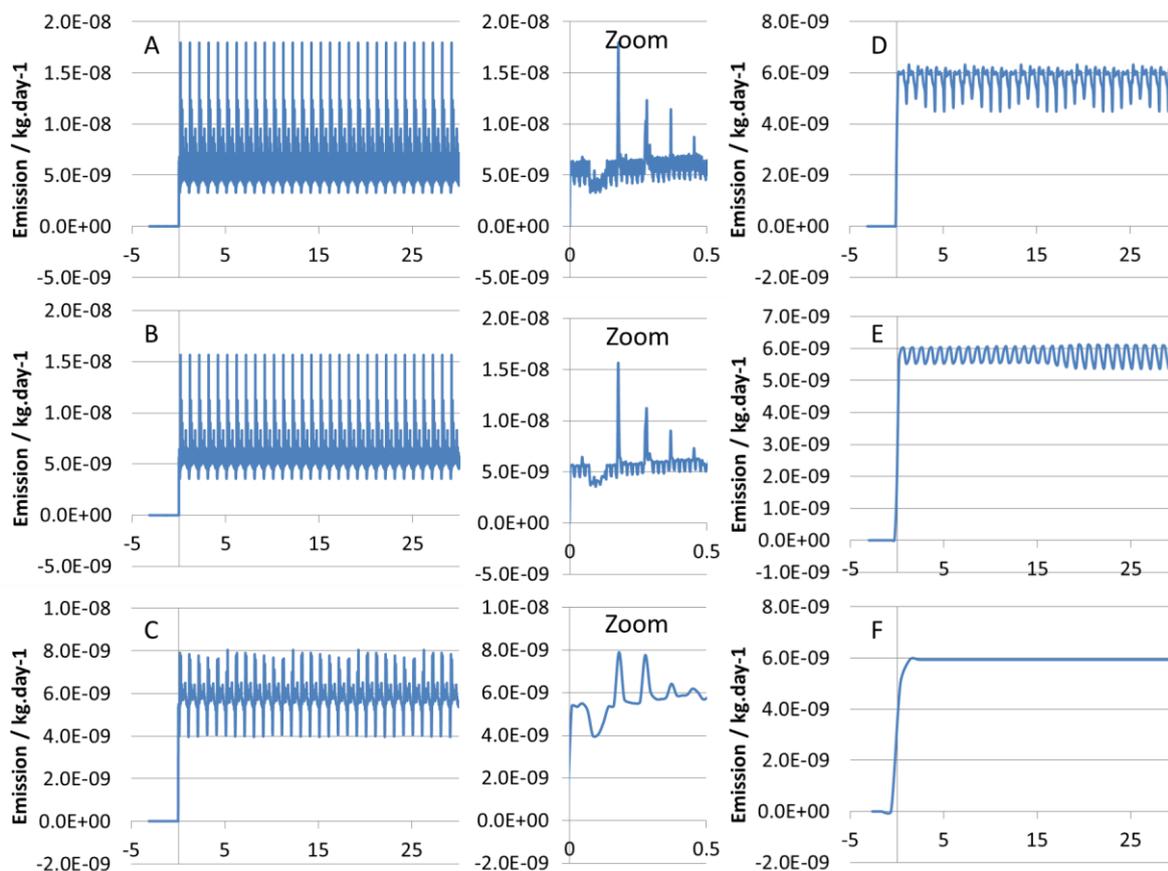


Figure V.6 – Chloroform emission by the life cycle system of a WWTP. The dynamic inventory was calculated for different time step sizes (A - 0.5 day, B - 1 day, C - 1 week, D- 1 month, E- 1 season and F- 1 year) and zooms are presented for the time between 0 and 0.5 years in A, B and C.

Chloroform emission is directly linked to the effluent flow, which presents seasonal effects during the year. The maximum amplitude of the emissions is observed for the smallest time step (0.5 days) in Figure 6.A. It ranges between $4\text{E-}9$ and $1.8\text{E-}8$ $\text{kg}\cdot\text{day}^{-1}$.

Figure V.7 shows the results for the current ecotoxicity, $n_{\text{eco}}(t)$, and human toxicity, $n_{\text{human}}(t)$, calculated over 100 years with the dynamic approach. All substances selected for the case study were considered for toxicity assessment. Different time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year) were used in the calculation of the dynamic inventory, which is the input to the dynamic toxicity model. The time step size used to retrieve toxicity results (from the toxicity model calculation) was the lowest one investigated, i.e. 0.5 day.

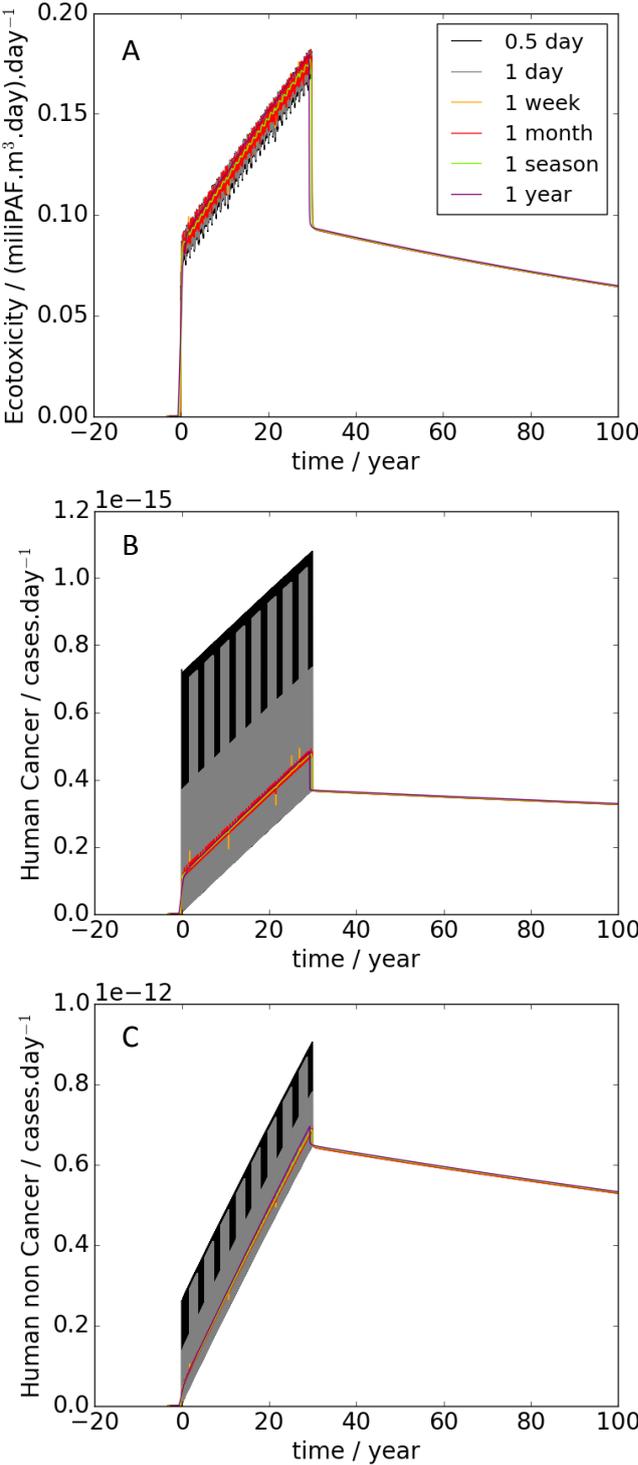


Figure V.7 – Ecotoxicity (A), human cancer toxicity (B) and human non-cancer toxicity (C) for the case study (all substances) calculated over 100 years, for different time step sizes in the LCI.

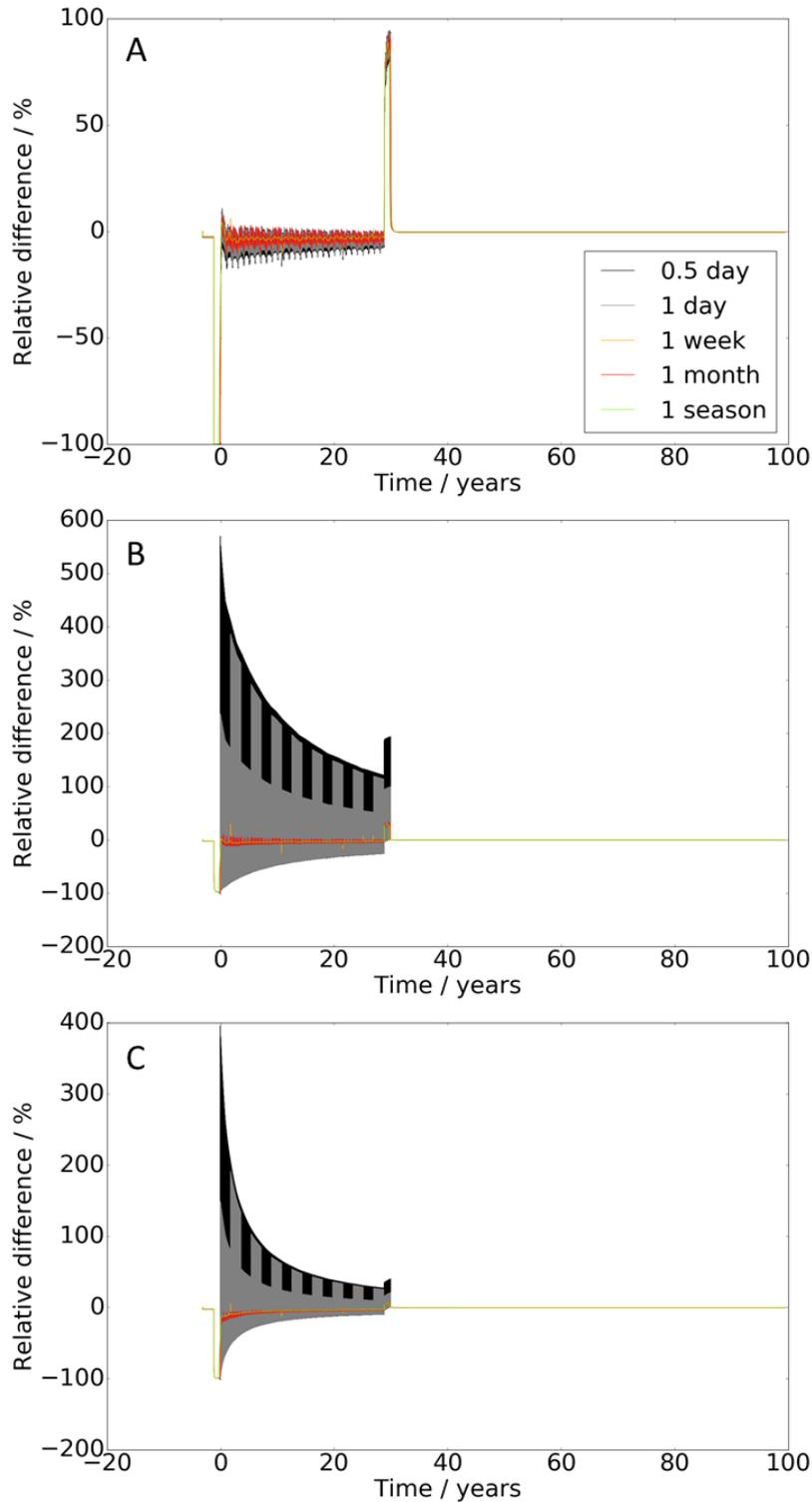


Figure V.8 – Relative difference for current ecotoxicity (A), human cancer toxicity (B) and human non-cancer toxicity (C), calculated with the dynamic approach for a time span of 100 years. Reference step size = 1 year. Step sizes analysed: 0.5 day, 1 day, 1 week, 1 month and 1 season.

Ecotoxicity results present slight differences between the amplitudes and temporal profile of the impacts calculated with different step sizes. The difference of amplitudes is much greater for both cancer and non-cancer human toxicity results. The observed differences of amplitudes and temporal profiles in the dynamic toxicity results are the direct reflection of the substance emission behaviour of the life cycle system and thus of the dynamic LCI. This aspect has already been pointed out by Shimako et al. (2017).

Figure V.8 shows the relative difference between the results for dynamic toxicity (all substances) calculated with different step sizes compared with the reference result (step size of 1 year). The most spectacular differences are observed for human toxicity. The profiles calculated for 0.5 and 1 day present significantly higher amplitudes than those obtained with other time step sizes. The relative difference for ecotoxicity is much smaller. Two distinct high amplitudes were obtained, one by year 0 and the other by year 30 but this is, in fact, an artefact attributable to the numerical integration method (Equation V.14).

Table V.4 shows the results of dynamic cumulated toxicity at 100 years, and the relative difference with respect to the conventional LCA results. In a previous study (Shimako et al., 2017), it was demonstrated that toxicity impacts due to non-persistent (organic) and persistent (mostly inorganic) substances had very different temporal profiles. For that reason, in the present work, calculations were performed considering all substances, or only organic substances, or only inorganic substances.

Differences between the dynamic approach and conventional LCA are very significant for “all substances” and “inorganic substances”, reaching 85% in the human cancer toxicity category. In contrast, relative differences are insignificant for “organic substances” et the chosen time span of 100 years. The concentration of non-persistent organic substances in all environmental media tends to zero by year 100, while inorganics persist and generate more and more cumulated impact. As conventional LCA considers steady state conditions (theoretically reached for constant emissions over very long time frames), i.e. an infinite time horizon, the conventional toxicity method overestimates the effect of inorganic substances. The dynamic approach provides much more realistic results at a given moment on the time scale. Indeed, the contribution of sink reservoirs in the Simplebox model (substance degradation and removal) is much more influent in real systems and dynamic conditions (emissions taking place over a limited duration) as in the theoretical “ideal” condition of continuous constant emission over infinity.

Moreover, the LCI time step size is not a sensitive parameter when the dynamic and conventional results are compared since the observed gap is dominated by the predefined time horizon of infinity.

It can be concluded that current dynamic toxicity exhibits a temporal profile with marked variations and large amplitude differences when distinct LCI time step sizes are used. For all toxicity categories,

the relative difference (between curves with different time step sizes) vanishes after the life time of the system, i.e. 30 years. At 100 years, the values of cumulated dynamic toxicities, calculated with different LCI time step sizes, are much the same (the relative differences between the reference case and the others do not exceed 1.7% - see SI V). The temporal variation of the potential toxicity impact ($\text{cases}\cdot\text{day}^{-1}$) and thus the most relevant point in time for the assessment is information that is inaccessible in the conventional method.

Table V.4 – Cumulated values for dynamic toxicity impact calculated over 100 years and values for conventional LCA (cLCA). Relative difference between dynamic and conventional results is given in parentheses.

All substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m ³ .day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.2E-11 (85.3%)	7.8E-11
human non – cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08
Organic substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m ³ .day)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.3%)	2.8E-06 (-0.6%)	2.8E-06 (-1.1%)	2.7E-06
Human cancer (cases)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.2%)	3.7E-14 (0.1%)	3.8E-14 (0.6%)	3.7E-14
human non – cancer (cases)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.0%)	1.4E-13 (0.4%)	1.4E-13 (0.8%)	1.4E-13
Inorganic substances							
	0.5 day	1 day	1 week	1 month	1 season	1 year	cLCA
Ecotoxicity (PAF.m ³ .day)	3.1E+00 (56.5%)	3.1E+00 (56.5%)	3.1E+00 (56.4%)	3.1E+00 (56.4%)	3.1E+00 (56.2%)	3.1E+00 (55.8%)	7.1E+00
Human cancer (cases)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.6%)	1.1E-11 (85.5%)	1.1E-11 (85.4%)	7.8E-11
human non – cancer (cases)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.9%)	1.7E-08 (80.8%)	1.7E-08 (80.8%)	1.7E-08 (80.6%)	8.9E-08

V.4.2. Influence of the time step of the dynamic impact model resolution

Climate change

The variation on the dynamic LCI step size (section 3.1) showed that there was no significant difference in the climate change results, for the mean temperature change, when calculations were performed with time steps from 0.5 day to 1 year. Using a 1 year step size for the inventory allows different step sizes (less than 1 year) to be used for the calculation of the dynamic climate change impact. The calculation was done for the dynamic LCIA step size of 0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year.

The three main GHG were considered in this analysis (carbon dioxide, methane and dinitrogen monoxide). A time step greater than 1 year was not envisaged in the present case study as it would have neglected some discrete mass values from the dynamic inventory.

Table V.5 shows the relative difference between the results obtained for the mean temperature change with different time step sizes. The relative difference is not significant for step sizes in the interval of 0.5 day to 1 season. However, the result obtained with a step size of 1 year shows differences of about 5%. Considering that the smallest time step size gives the most precise results, this means that any step between 0.5 days and 1 season can be used, given the insignificant difference between the results.

Table V.5 – Relative difference for mean temperature change, obtained for different time step sizes in the climate change model resolution.

Relative difference for ΔT	0.5 day	1 day	1 week	1 month	1 season	1 year
0.5 day	0.0%	0.0%	0.0%	-0.1%	-0.4%	-5.2%
1 day	-	0.0%	0.0%	-0.1%	-0.4%	-5.2%
1 week	-	-	0.0%	-0.1%	-0.4%	-5.1%
1 month	-	-	-	0.0%	-0.3%	-5.0%
1 season	-	-	-	-	0.0%	-4.8%
1 year	-	-	-	-	-	0.0%
Calculation time	9h 34m 30s	2h 23m 20s	3m	15s	6s	8s

In this work, a personal computer with an Intel Core i5-2540M processor at 2.60 GHz and 4 GB of RAM was used. Even though the computer can support multithread, only a single core was used for the computation. The calculation time decreased substantially when the step size for the convolution calculation was increased, because of the number of iterations required by a convolution product (Garge and Shirali, 2012):

$$\text{iterations} = \frac{\text{number of discretizations} (\text{number of discretizations} + 1)}{2} \quad \text{Equation V.17}$$

As the difference between the results is not substantial, a time step size of 1 month or 1 season could be envisaged for the calculation and would provide a good compromise between accuracy of results and computational efficiency.

Toxicity

A similar comparison between different step sizes was not possible in the dynamic toxicity model because the dynamic toxicity results are, first of all, very sensitive to the time step size of the inventory. Calculation of dynamic toxicity using a 1 year step size for the dynamic inventory is not suitable as it does not consider all the potential variations and amplitudes of the toxicity impact. Moreover, it has been shown (Shimakoto et al., 2017) that the resolution of the dynamic toxicity model depends on the resolution of an ODE, which requires an adaptive integration time step. Thus, the lower the time step is, the more reliable is the dynamic impact profile and the more accurate is the numerical resolution. It is, however, possible to set the maximum step for the ODE solver in the toxicity model at the LCI step size, e.g. 0.5 days.

V.5. Conclusion

The dynamic LCA framework presented here combined the DyPLCA inventory model with dynamic climate change and dynamic toxicity impact assessment models. Sensitivity analysis was conducted on a case study in order to identify the influence of the temporal profile of the dynamic LCI and the time horizon on the final LCA results. Additionally, parameters of numerical methods used for the resolution of the impact models were investigated.

As a general remark, both impact categories exhibit high variation over the calculation period (100 years in this study), which cannot be captured in a single impact value at a given time (or a fixed time horizon), e.g. 100 years. Instead, a detailed analysis is necessary during the first few decades. In this case, a graphical representation of the LCA results is of great interest for the identification of the general temporal profile.

The subsequent conclusion is that a fixed time horizon, as implemented in conventional LCA, deprives us of essential information, especially for short and medium time periods corresponding to the lifetime of the studied system and about the following twenty years.

For climate change impact, two dynamic indicators were analysed: the global mean temperature change and the cumulated radiative forcing. The temporal profile of both indicators depends on the target substance and the global positioning of the GHG emissions on the time scale, i.e. emission beginning and duration. In consequence, a fixed time horizon as in conventional LCA is highly arbitrary and does not correspond to any point of interest on the time scale of the processes, i.e. temporal LCI and dynamic phenomena involved in impact deployment.

In this work it is shown that neither dynamic indicator is sensitive to the level of detail of the temporal LCI definition. Simulations performed for the same process system, but varying the granulometry of the LCI from 0.5 day to 1 year, led to similar results.

The dynamic climate change model is not sensitive to the change of time step size for numerical resolution, on condition that it lies below the LCI time step size (otherwise inventory information can be lost). For the case study, a time step of 1 month satisfied the resolution accuracy condition, for a very reasonable computational effort.

The dynamic toxicity model was based on USEtox[®] model parameters. As in the case of climate change, the toxicity temporal profile depends on the target substance and temporal definition of LCI. However, unlike for climate change, in the case of toxicity, the level of detail of the LCI definition (time granulometry) has a major influence on the results: toxicity results are highly sensitive to the LCI time step. Concerning the time span of calculation, as in the case of climate change, there is no justification for fixing a predefined value. In conventional LCA, the fate of substances in the environment is considered to be at steady state, i.e. the time horizon is infinite and sink processes are compensated by the continuous infinite emission. However, it is shown here that the most interesting period is the lifetime of the studied system, i.e. the emission duration, and several decades afterwards.

In the toxicity dynamic model, a finer time grid is necessary in order to capture the inventory information and for the resolution of the ODE system. The maximum time step could be set at the lowest LCI time step (e.g. 0.5 days).

Acknowledgments

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Case study: French electricity mix for the period between 2010 and 2070

V.6. Introduction

The Renewable Energy Directive (RED) establishes national energy targets for countries in the European Union (EU). They envisage decreasing the emission of greenhouse gases through the implementation of renewable energy sources. In November 2016, a revision of the directive envisaged a target of at least 27% of renewable energies for the European Union by 2030. In France, a target of 23% of renewable energies in the total energy consumption is envisaged for 2020 (RED, 2016).

France has a significantly low-carbon electricity mix due to the use of nuclear energy. However, the lifetime of several nuclear plants in France already reached 30 years which is close to their foreseen lifetime of 40 years. The choice to extend the lifetime of nuclear power plants or replacement by other plants has been questioned (IEA, 2017).

During the last years, French government is looking forward for solutions in order to have more secure, affordable and sustainable energy (IEA, 2017). Giving the aging of the nuclear energy infrastructure and the fact that cost of renewable energy has been decreasing over the last years, the French government set ambitious targets to diminish the share of nuclear energy for the upcoming years replacing it by green sources of energy (IEA, 2017)

The French environment and energy management agency (ADEME) presented different scenarios to describe the future of electricity production in France. They describe three different scenarios which depend on the choice of maintaining or not nuclear energy (ADEME, 2013).

Regarding the objective of decreasing the emission of greenhouse gases, different studies about the carbon emission of these scenarios were developed. However, those results provide only steady state and single values of CO₂ equivalent emission which do not represent all the climate change aspects of these systems. The response of the environment has its own dynamics which are not accounted in the conventional approach. Also, other impacts related to the change of the electricity mix are not accounted.

The objective of this study is to evaluate temporal dimension influence on the environmental impacts due to the choice of electricity sources for the French mix. The period analysed is between the years 2010 and 2070. Two different impact categories are analysed: climate change and toxicity.

V.7. Case study: French electricity mix for a sustainable future

A case study considering the scenarios of electricity mix in France from 2010 to 2070 was chosen to apply the complete framework of a dynamic LCA

V.7.1. Goal and scope definition

The objective of this LCA case application is to analyse the potential environmental impacts due to the choice of keeping or not nuclear energy in the future French electricity mix scenarios. The dynamic approach is compared with the results obtained by the conventional LCA method.

The unit function was 1kWh of electricity consumed in France between the years 2010 and 2070. The French mix is distinct in three different periods which are divided evenly during the period of analysis (from 2010 to 2030; from 2030 to 2050; and from 2050 to 2070).

Systems boundaries for the chosen functions were as large as possible (cradle to grave) which relies in the data from the ecoinvent 3.2 database. Default allocation method was chosen in this database.

The LCA software Simapro[®] 8.2 was used for the calculation of conventional LCA as well as the technological and environmental matrices for use in the dynamic life cycle inventory (DLCI) step. Moreover, Dynamic LCI was calculated with the DyPLCA web platform (<http://dyplca.univ-lehavre.fr/>) and dynamic DLCIA was calculated with the Python tool developed in this study (chapter III, IV and V).

V.7.2. LCI

Table V.6 shows the information about French electricity consumption and electricity mix for different periods of time: 2010-2030; 2030-2050 and 2050-2070 (high and low nuclear energy scenarios).

According to ADEME (2013), the electricity consumption in France will be stable for the next years. The consumption in the period of 2010-2030 is estimated at 38.1 Mtep per year. For the other periods the predicted consumption is around 31 Mtep per year. Nevertheless, even though the consumption will not decrease considerably, the major change in the electricity mix in France can provide better environmental results due to the use of renewable energies.

Current electricity scenario is based on data from the service of data and statistical studies (SDES) from the Ministry of Ecological and Solidarity Transition (MEST, 2017). Nuclear energy is the major source of electricity for the current mix presenting a contribution of 77% for the mix. The main infrastructure technology for nuclear energy used in France is “pressurised water reactor (PWR) (IEA,

2017). Hydroelectricity was the renewable energy the most used in 2010 contributing with 12% to the mix.

Table V.6 – French electricity mix for different periods: 2010-2030; 2030-2050 and 2050-2070 (high and low nuclear energy scenarios)

Process	Consumption prediction (Mtep per year)	Electricity source	Mix contribution (%)
French mix 1 2010 – 2030	38.1	Coal	3.3
		Oil	1.1
		Natural gas	2.0
		Wind	2.7
		Hydro	12.1
		Photovoltaic	0.7
		Nuclear	77.3
		Biogas	0.2
		Waste incineration	0.2
		Wood	0.2
		Geothermal	0.1
		Sea	0.1
French mix 2 2030 – 2050	30.7	Wind	23.8
		Hydro	11.2
		Photovoltaic	9.6
		Nuclear	51.6
		Biogas	0.2
		Waste incineration	1.0
		Wood	1.0
		Geothermal	0.3
French mix 3 2050 – 2070 (high nuclear scenario)	30.9	Wind	22.9
		Hydro	10.7
		Photovoltaic	9.2
		Nuclear	49.5
		Biogas	5.1
		Waste incineration	0.6
		Wood	0.6
		Geothermal	0.3
French mix 3' 2050 – 2070 (low nuclear scenario)	30.9	Wind	34.8
		Hydro	14.7
		Photovoltaic	15.9
		Nuclear	19.1
		Biogas	5.2
		Waste incineration	0.6
		Wood	0.6
		Geothermal	0.6
Sea	10.0		

ADEME (2013) proposed different scenarios for years 2030 and 2050 for metropolitan France. Fossil source of electricity was considered to be completely replaced by other electricity sources, renewable for instance. For this study, the mix of year 2030 was considered stable for the period between 2030 and 2050 and the mix for year 2050 was considered lasting for the period between 2050 and 2070.

For 2030, ADEME (2013) expected the French electricity mix to be composed by around 50% of nuclear energy. The main source of renewable energy should be the wind that will have a contribution of more than 23%.

ADEME (2013) proposed three different scenarios for 2050 which are based on the use of nuclear energy: high, medium and low. The high nuclear electricity consumption scenario considers that the contribution of nuclear energy for the French mix will not change with respect to 2030. The medium nuclear energy scenario considers that half of nuclear energy is replaced (i.e. a contribution of 25%). And finally the low scenario considers that nuclear energy will represent only about 20% of the total electricity mix. High and low nuclear utilisation scenarios were analysed and compared in this study.

All necessary data for the LCI building were taken from ecoinvent 3.2, considering that the technologies for electricity production do not change over the calculation period (i.e. the same dataset is used for a given product).

The case study was first implemented in Simapro[®] software with the 3 mix types defined as “mix” activity, i.e. a proportion of each electricity type and no direct emissions or resource consumptions (like a “market” activity). The foreground (reference unit 1kWh) is thus composed of 0.38 mix1+0.31 mix2 + 0.31 mix3 (or 3’). The background processes, i.e. electricity production by different technologies and the back linked processes were taken from ecoinvent. From now on, the scenario which presents the lowest share of nuclear energy will be called low nuclear scenario and the other high nuclear scenario.

V.7.3. Dynamic LCI

The mix was considered to be constant over a given period of time. Mix activities are considered like “market” activities, as explained above. The temporal parameters of these 3 “mix” activities are thus very simple: constant production (alpha function), no emissions (b_{ii} and b value in beta are zero), life period T of 20 years (the mix period).

In order to place the 3 mix types consecutively in time, the delta parameter was defined as a delay with respect to the t_0 of the reference unit (table VI.2.2 in SI). Supply of electricity for the mix is considered to be continuous and constant.

The temporal parameters for electricity processes and all background processes were previously defined in the temporal database developed in DyPLCA project and taken as such in this application. Considering the electricity process in the background, delay of electricity supply is zero as there is no storage of electricity. Also, the representative period/infrastructure lifetime varies depending on the source of energy.

The matrixes A and B of the case study were exported from Simapro[®] and imported to DyPLCA tool. The results of the dynamic LCI were then used for dynamic impact calculation.

V.7.4. LCIA

The impact categories chosen in this study are those for which a dynamic approach exists, as presented in section 2.1. The IPCC climate change and USEtox[®] toxicity models are at the basis of the dynamic impact models and were also used in conventional LCA applied to the case study.

A calculation time span of 100 years was chosen for both dynamic impacts. In conventional LCA, a time horizon of 100 years is commonly used for climate change while for toxicity categories steady-state condition is imposed for substance fate in environment.

V.8. Results and discussions

V.8.1. Inventory

Both dynamic LCI scenarios comprised 10104 activities and 2406 environmental interventions. Production systems are composed by 226307 supplies between activities which generate 344888 environmental interventions associated to the processes of the supply chain. A threshold value is used in order to limit the calculation time for the graph search algorithm to a relative value of 1E-4 for the material balance. This value allowed the consideration of more than 80% of all products and elementary flows, for both scenarios. Decreasing the threshold value leads to a better coverage of the material flows but the calculation time would increase significantly. The time of calculation for each scenario was around 9h.

Considering the time scale for LCI calculation, the time zero was set to 1st January 2010. The period 2010-2030 was then represented by the time between 0 and 20 years; 2030-2050 was represented by the time between 20 and 40 and finally the period 2050-2070 was represented by the time between 40 and 60.

V.8.2. Climate change assessment

For dynamic climate change impact, 66 combinations substances/compartment/subcompartment, were considered for each scenario.

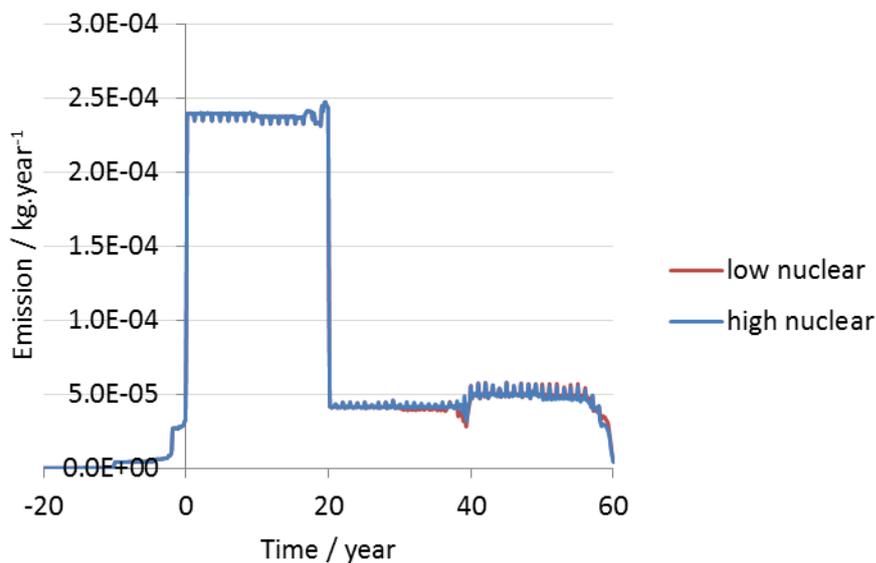


Figure V.9 – Emission profile for “carbon dioxide in air, low pop.” for scenarios low and high nuclear energy scenarios.

Figure V.9 shows the emission profile for “carbon dioxide in air, low pop.” in low and high nuclear energy scenarios. This GHG has important contribution to dynamic climate change impact (SI VI). When calculating the dynamic radiative forcing, this substance had the major contribution for the cumulated values at year 100. The three zones corresponding to the periods of distinct electricity mixes are distinguishable on this figure. The emission level for the first period (2010-2030) is significantly higher than for the other two periods due to the presence of fossil fuel based electricity. Also, no important noise (variations) was observed as the carbon dioxide is mainly a direct emission of the electricity production process which supply is continuous. Finally, the emission profile for both scenarios is very similar for all periods of evaluation.

Figure V.10 shows the results of global mean temperature change and cumulated radiative forcing for low and high nuclear energy scenarios. Cumulated radiative forcing (B) increased until year 100 for both scenarios. Moreover, even though the slope of the curve might decrease, the curve profile will never reach a constant value as the airborne fraction of carbon dioxide will keep contributing to the impact until infinite.

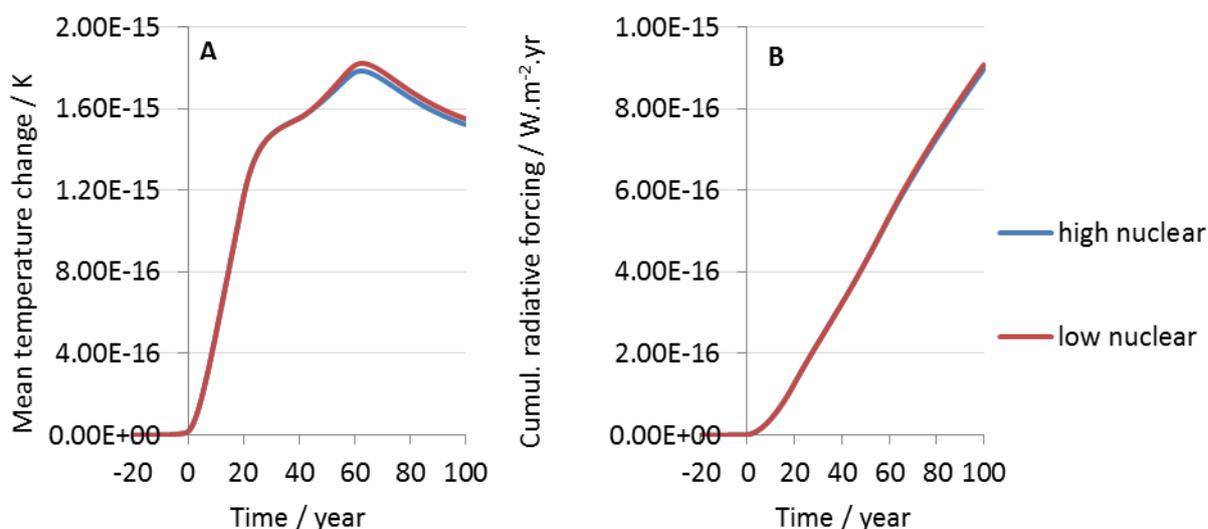


Figure V.10 – Dynamic mean temperature change and cumulated radiative forcing calculated over 100 years for scenarios low and high nuclear for the French electricity mix.

In the case of mean temperature change (A), the maximum value of $1.8\text{E-}15$ is reached at year 62 for both scenarios. This value is neglected in the conventional method as only a certain value at a time horizon is given. Also, almost no difference could be seen between the results for scenario low and high nuclear energy scenarios.

Table V.7 shows the value of cumulated radiative forcing and mean temperature change at year 100 and the conventional LCA values (time horizon of 100 years).

Regarding the conventional radiative forcing values, they can be obtained by multiplying the impact result in $\text{kgCO}_2\text{-eq}$ by the AGWP100 of CO_2 ($9.17\text{E-}14 \text{ Wm}^{-2}\text{yr}$) (IPCC, 2013).

Table V.7 – Dynamic mean temperature change and cumulated radiative forcing results for 100 years for low and high nuclear scenarios for the French electricity mix.

Scenario	Conventional climate change ($\text{CO}_2\text{-eq}$)	Conventional radiative forcing (Wm^{-2})	Dynamic radiative forcing (Wm^{-2})	Dynamic mean temperature change (K)
High nuclear electricity mix	0.013	$1.2\text{E-}15$	$8.9\text{E-}16$	$1.5\text{E-}15$
Low nuclear electricity mix	0.014	$1.3\text{E-}15$	$9.0\text{E-}16$	$1.6\text{E-}15$

The results of radiative forcing for the dynamic method were lower than for the conventional method. Given the distribution of emission over time in the dynamic model, the impacts are delayed compared to the conventional method which considers all emissions at time zero. The dynamic method accounts more realistically the potential impact than the conventional method with respect to the time scale.

Mean temperature change (in conventional method is called GTP) is not available in Simapro[®], for this reason, no conventional result is given. Both the conventional and dynamic methods give quite similar values for climate change indicators for high and low nuclear energy mix; there is no difference between these scenarios with respect to climate change impact.

Regarding the process contribution analysis (SI VI.4), the main contribution to climate change impact (GWP100) is obviously related to fossil fuels consumption with special attention to electricity production from hard coal. These processes are only present in the period 2010-2030. As the mix and the quantities of energy for the period 2010-2030 are the same for both scenarios, no difference can be seen between the results. The mix technologies used in the period 2050 - 2070 have low carbon emission which leads to the almost the same results for climate change.

V.8.3. Toxicity assessment

Dynamic toxicity impact calculation considered 742 substances/compartment/subcompartment sets from the inventory, for each scenario.

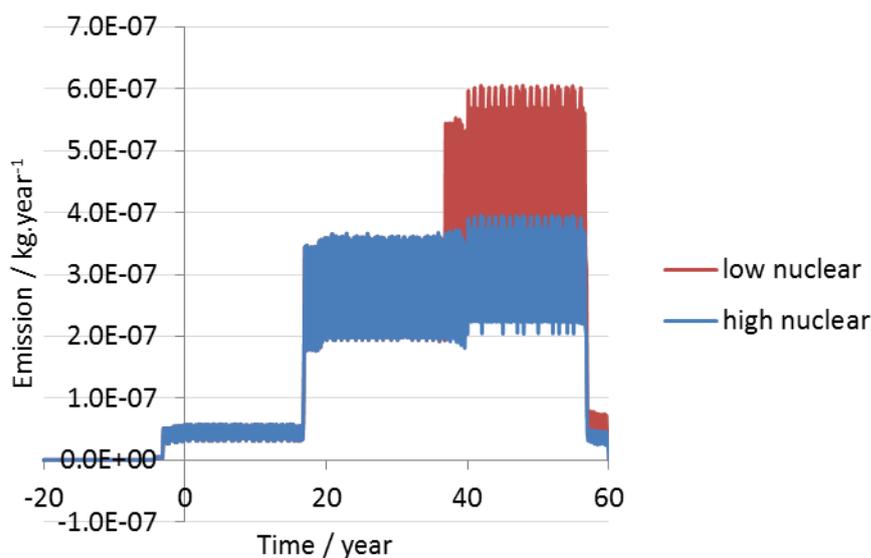


Figure V.11 – Emission profile for “copper in. water, groundwater, long-term” for low and high nuclear energy scenarios.

Figure V.11 shows the emission profile for “copper in water, groundwater, long-term” for low and high nuclear energy scenarios. This substance was chosen due to its important contribution to dynamic freshwater ecotoxicity impact (SI VI). The figure shows three distinguishable zones corresponding to the periods of different mixes. The highest values of emissions are observed in the last two periods (between 2030 and 2070). Moreover, an important increase of the emission is observed for the period 2050-2070 (between year 40 and 60) for low nuclear scenario. This scenario presents a higher emission of “copper, in water, groundwater, long-term” due to the composition of its electricity mix. For the periods between 2010 and 2050 (from 0 to 40 on the graph), the emission profile is similar for both scenarios. The profile of emission presents an important degree of noise which means that the main processes releasing this emission do not have a continuous supply. As all foreground processes are electricity production processes with continuous distribution, this profile can be attributed to background processes.

Figure V.12 shows the current values for eco and human toxicity for low and high nuclear energy scenarios. By year 100, the existence of a great share of impact which decreases slowly is the main evidence of the great influence of metals. For example, the contribution of “copper in water, groundwater, long-term” explains this dynamic profile for the ecotoxicity category. On the other hand, human cancer toxicity (B) is mainly determined by organic substances (benzo(a)pyrene, air, low population) given the noisy profile of impacts between the years 0 and 60 and the fast decrease after the end of the emissions (after year 60). Metal also contribute to this impact category, as shown by the tail at long term in figure B (mainly chromium VI, air, low population, and air low population long-term). The non-cancer toxicity is mainly determined by persistent inorganics (cadmium, air, low population). The major share of the impact is concentrated between the years 0 and 60. The results for ecotoxicity and human toxicity non-cancer started to differ at year 40 when the two scenarios start to present different sources of electricity. Low nuclear electricity scenario shows higher values for ecotoxicity from year 40 and the difference reach a constant value around year 60.

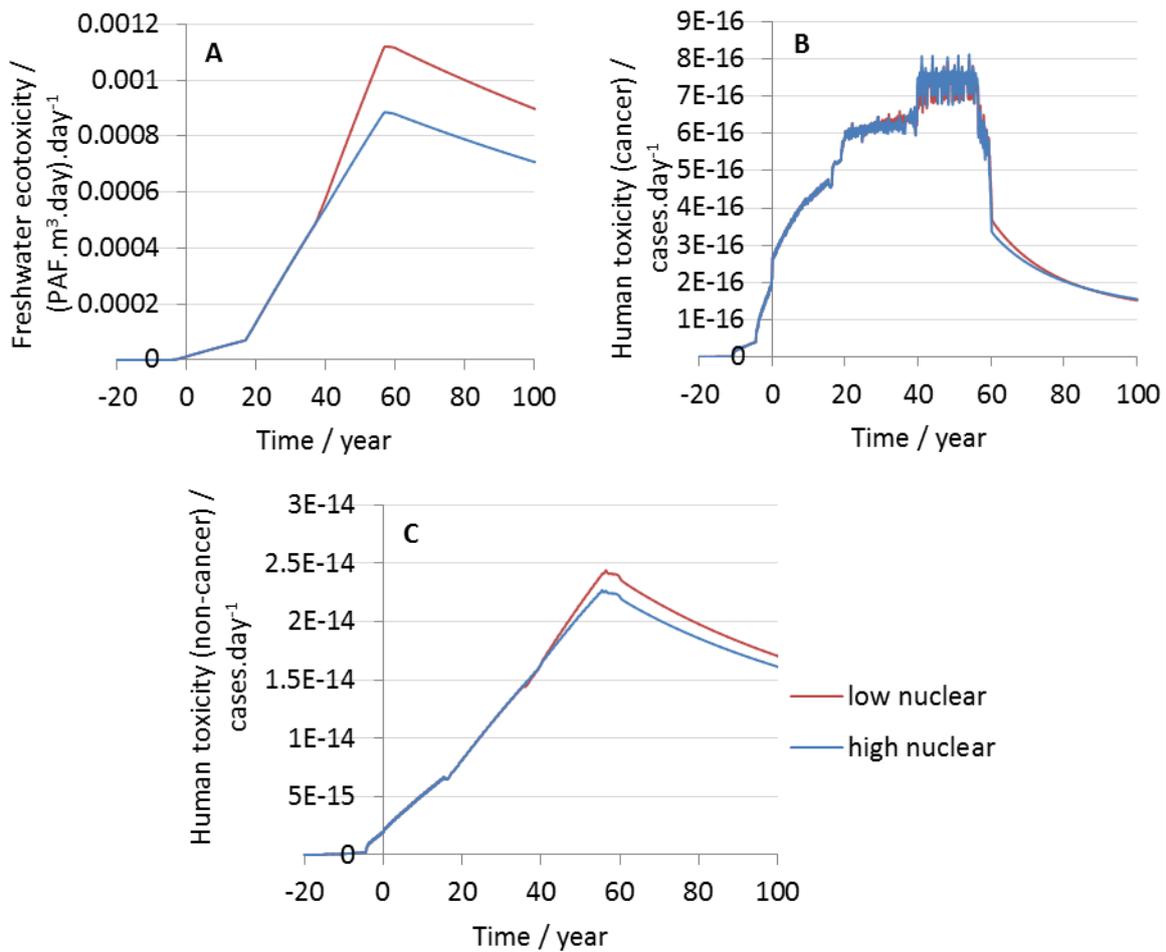


Figure V.12 - Current dynamic toxicity impacts calculated for the French electricity mix for low and high nuclear energy scenarios. A – Freshwater ecotoxicity, B – Human cancer toxicity and C – Human non-cancer toxicity.

Figure V.13 shows the cumulated values for eco and human toxicity for low and high nuclear energy scenarios. The results for human toxicity (B and C) show that almost no difference exists between scenarios. For freshwater ecotoxicity (A), the ratio high/low nuclear energy at year 100 is around 94%, i.e. the difference is of low significance.

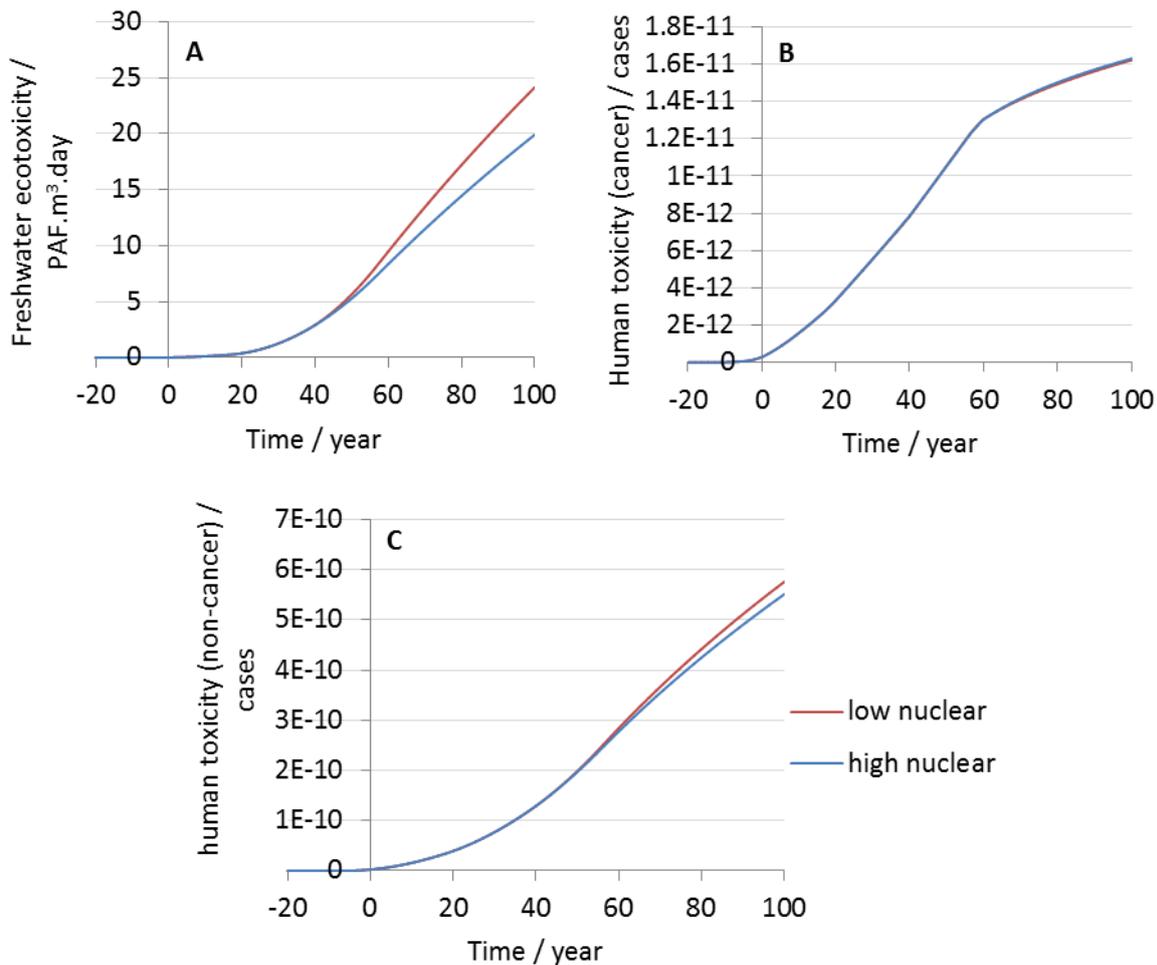


Figure V.13 – Cumulated dynamic toxicity calculated over 100 years for low and high nuclear energy scenarios. A – Freshwater ecotoxicity, B – Human cancer toxicity and C – Human non-cancer toxicity.

Table V.8 shows the results for conventional and dynamic toxicity for low and high nuclear energy scenarios. Conventional toxicity was calculated with the characterization factors provided by USEtox[®] 2. Conventional and dynamic impacts results show important differences, the presence of inorganic substances being the main reason for the distinct results. Organic substances tend to be rapidly removed from environment, their potential impact is limited to the emission period and their low residence time, which would lead to similar results between conventional and dynamic methods (as discussed in chapter IV. In conventional evaluation, ecotoxicity was the impact category which presented the highest difference between scenarios.

Table V.8 –Conventional and dynamic (span time of 100 years) cumulated toxicity impacts for high and low nuclear scenarios for the French electricity mix.

Scenario	High nuclear electricity mix (A)	Low nuclear electricity mix (B)
Conventional ecotoxicity (PAF.m ³ .day)	69.2	86.5
Dynamic ecotoxicity (PAF.m ³ .day)	19.9	24.1
Conventional human cancer toxicity (cases)	1.3E-8	1.3E-8
Dynamic human cancer toxicity (cases)	1.6E-11	1.6E-11
Conventional human non-cancer toxicity (cases)	4.0E-8	3.9E-8
Dynamic human non-cancer (cases)	5.8E-10	5.6E-09

A contribution analysis in Simapro[®] using USEtox[®] 1.04 was performed (details in SI VI.4) (Usetox 2 is not available in Simapro 8.2). The results cannot be directly compared with the results of Table V.8 given the differences between USEtox[®] versions. However, the contribution analysis can give indications about the influence of processes on the impacts. The treatment of scrape copper from municipal incineration was the main contributor for ecotoxicity. It is linked to the waste treatment of the infrastructure of wind power plants. These impacts should have appeared later in the assessment (i.e. at year 2070 for the infrastructures starting at year 2050). However, they were distributed over time as services/usual activities as the infrastructure processes are not sufficiently detailed in ecoinvent and not yet well defined in the dynamic LCI model (see chapter II).

In ecoinvent, processes related to infrastructure construction and dismantling are linked directly on the same functional reference flow e.g. one building. This database structure is an important limitation when implementing a dynamic approach. In the dynamic approach, the processes are separated in time due to the network – graph structure. The construction of this temporal structure is based on ecoinvent technological matrix and thus depends on the degree of aggregation of processes in ecoinvent.

In conventional human toxicity, the difference between the results of scenarios is not significant. The major contribution for all conventional toxicity categories comes from *waste treatment* activities. In non-cancer human toxicity category, the process with major contribution is the treatment of uranium tailing which is a waste of uranium milling. Considering cancer human toxicity, the results are very similar as the major contribution comes from the treatment of slag from the incineration of waste. This process has almost the same percentage of contribution in both scenarios.

V.9. Case study conclusions

The complete dynamic LCA framework was successfully applied on a case study concerning the French mix in the period of 2010 to 2080. This study showed the outcomes and limitations of the complete framework including the dynamic LCI with the integration of the temporal database, and dynamic LCIA.

Regarding the web platform DyPLCA for the calculation of dynamic LCI, the integration with the database was successfully done. The coverage of the network by the graph model was satisfactory reaching more than 80% of all processes and emissions. The three different periods of emission was well distinguishable and correspond to the expected profile, except the lack of correct temporal parameters for infrastructure disposal processes.

The scenarios for high and low use of nuclear energy in the mix exhibited no significant differences for climate change. The change in the electricity mix will not have huge influence in the decrease of carbon emissions policy. Considering the calculation of toxicity, freshwater ecotoxicity presented the highest difference due to the waste treatment which comes from the use of wind-based energy. Moreover, the possible improvement of the environmental performances cannot be based only on these two impact categories. An important aspect to be evaluated is the waste management of radiative material which is not fully and accurately covered by toxicity impact category.

Using the dynamic method showed that the conventional method usually overestimate the results as the emissions are all accounted at time zero. The distribution of emission over time gives a completely different perspective of impacts. Also, the results and the profile of the impacts in the dynamic assessment undergo the influence of the nature of the substance.

Chapter VI. Conclusions and perspectives

Conclusions [FR]

Ce travail de thèse a permis le développement d'outils pour la mise en place d'une méthode ACV dynamique. Les outils et méthodes développés permettent l'application de l'ACV dynamique par les praticiens d'ACV sans avoir à gérer des changements radicaux par rapport à la méthode conventionnelle.

Au niveau de l'ICV dynamique, ce travail a apporté une contribution pour le développement d'une base de données des paramètres temporels pour les processus et les chaînes d'approvisionnement. Cette base de données temporelle associée à ecoinvent v3.2 est nécessaire pour construire le réseau/système de processus et résoudre le modèle d'ICV dynamique pour l'arrière-plan de tout système de produits. Cette étude a contribué avec des données pour les processus chimiques et biologiques existant dans ecoinvent. De plus, une analyse approfondie des procédés ecoinvent a permis des propositions d'amélioration du modèle d'ICV dynamique général. Plusieurs propositions ont déjà été implémentées dans l'outil web DyPLCA.

Une approche dynamique a été proposée pour la catégorie d'impact du changement climatique, avec deux indicateurs: le forçage radiatif (instantané et cumulé) et le changement de température moyen. Les deux indicateurs ont une signification physique et sont impliqués dans la chaîne cause-effet du processus climatique. Les résultats d'impact sont obtenus en tant que valeurs d'indicateurs pour n'importe quel moment. Dans le cas du changement de température moyen, une valeur maximale est atteinte à un moment donné en fonction de la nature des GES et du profil d'émission. La méthode proposée est flexible car elle ne nécessite pas d'horizon temporel fixé, contrairement à l'ACV classique. Le choix d'un horizon temporel a priori est arbitraire car il ne reflète pas le comportement temporel du système de production étudié. La méthode n'utilise pas des facteurs de caractérisation (établis pour une émission impulsionnelle unitaire au temps zéro et pour un horizon temporel fixe), mais calcule les indicateurs d'impact en fonction de la charge atmosphérique réelle déterminée par un profil d'émission donné. De plus, une substance de référence n'est plus nécessaire. Un autre résultat de l'approche dynamique est la possibilité de comptabiliser tous les types de dioxyde de carbone, c.-à-d. fossiles et biogéniques, et d'évaluer la contribution réelle du CO₂ biogénique aux indicateurs climatiques. Une analyse de sensibilité réalisée sur un cas d'étude démontre que les indicateurs dynamiques sont sensibles à la durée et à la position dans le temps, mais les variations d'émission sur de courtes périodes (moins d'un an) ne sont pas déterminantes pour les résultats d'impact.

Une approche dynamique de l'évaluation de la toxicité a été également proposée dans ce travail. Ce modèle est basé sur le modèle USEtox[®] et utilise le modèle dynamique Simplebox pour le calcul du devenir de la substance en fonction du temps. Ainsi, le facteur du devenir disparaît et est remplacé par la distribution de la substance dans les compartiments environnementaux en fonction du temps. Les

facteurs d'exposition et d'effet sont inchangés et considérés comme constants dans le temps. Les indicateurs sont proposés pour la toxicité humaine (cancer, non-cancer) et l'écotoxicité d'eau douce. Les facteurs de caractérisation (obtenus en conditions stationnaires, émission continue et horizon temporel infini) ne sont plus nécessaires. Deux indicateurs sont calculés pour chaque catégorie d'impact: la toxicité actuelle en fonction du temps comme mesure du potentiel toxique instantané, et la toxicité cumulée en fonction du temps comme une mesure de l'ensemble des dommages comptabilisés à un moment donné.

Les substances organiques (non persistantes) et inorganiques (persistantes) ont des comportements très différents. Les substances organiques tendent à être éliminées relativement rapidement des compartiments environnementaux et leur devenir suit une évolution similaire au flux d'émission dans le temps. Les substances inorganiques sont pour la plupart persistantes et accumulées dans certains compartiments, leur potentiel de toxicité dure pendant des siècles. Ces caractéristiques ne sont pas mises en évidence dans les résultats d'ACV conventionnels. L'analyse de sensibilité réalisée sur un cas d'étude montre que la définition temporelle de l'ICV, c.-à-d. la caractéristique temporelle de l'émission d'une substance (durée, variation dans le temps, granulométrie temporelle), est déterminante pour l'impact toxicité. Les résultats de toxicité sont sensibles à la granulométrie temporelle d'un jour, c.-à-d. les variations des émissions sur une journée sont capturées par le modèle de toxicité et ont une répercussion sur les résultats de l'impact.

Enfin, le cadre de travail complet composé de la dernière version de l'application web DyPLCA connectée à la base de données temporelle, la base de donnéesecoinvent et le calcul dynamique des impacts, a été appliqué pour un cas d'étude du mix d'électricité français. Cette application démontre le fonctionnement de l'ensemble et la faisabilité de l'ACV dynamique.

L'outil d'ICV dynamique a fourni une bonne couverture de l'ensemble du système de produits de cycle de vie et s'est révélé satisfaisant par rapport aux résultats de l'inventaire conventionnel (le bilan massique final des méthodes dynamiques et conventionnelles devrait être similaire). De plus, toutes les émissions ont été correctement réparties dans le temps en fonction des paramètres temporels définis pour les procédés de premier plan et inclus dans la base de données temporelle (pour les processus d'arrière-plan). Concernant l'étape dynamique de l'EICV, les résultats obtenus pour les catégories d'impact changement climatique et toxicité ont montré les mêmes caractéristiques que celles discutées dans les chapitres dédiés.

Néanmoins, le développement d'une méthode d'ACV dynamique est encore au début. Plusieurs perspectives de développement sont mentionnées ci-dessous.

L'intégration de l'étape d'EICV à l'application web déjà existante faciliterait l'utilisation et permettrait aux praticiens de l'ACV d'utiliser efficacement l'approche développée sans exiger la manipulation des différents logiciels qui la composent.

Les cas d'études réalisés dans ce travail sont les seuls à ce jour, et concernent peu de domaines technologiques (comme procédés de premier plan). Multiplier les cas d'études dans différents domaines est nécessaire afin d'évaluer plus précisément les caractéristiques temporelles des procédés et des chaînes d'approvisionnement. Le CSTB et le LISBP étudient déjà les aspects dynamiques liés à la construction et à l'utilisation des bâtiments.

Les données temporelles pourraient être mises en œuvre par les contributeurs et les développeurs de bases de données d'ACV classiques qui sont les plus à même de collecter des informations pertinentes. L'ajout de caractéristiques temporelles dans la base de données temporelle suivrait la même procédure que l'entrée du flux de matières, les interventions environnementales, l'incertitude, etc.

Dans l'EICV dynamique, deux catégories d'impact ont été adaptées. Afin de fournir un large éventail de possibilités dans l'évaluation d'impact dynamique, il faut étudier davantage d'indicateurs afin de mettre en œuvre la dimension temporelle dans leur calcul. La déplétion de la couche d'ozone, l'acidification terrestre ou les rayonnements ionisants sont des exemples d'impacts qui ont des caractéristiques temporelles différentes.

“Every new beginning comes from some other beginning’s end.”

Seneca

Life Cycle Assessment is a widely accepted method for the environmental evaluation of anthropogenic activity. Moreover, LCA is standardized by ISO 14040-14044 which specify the guide for conducting a LCA study. The major feature of this method is the broad and complete evaluation of the impacts associated to products, processes and services over their entire life cycle

However, this method also has drawbacks which could be addressed and ameliorated. Among them, the lack of a temporal dimension is one of the issues less studied in the field. The absence of temporal characterization in life cycle inventory and life cycle impact assessment deprives us of important information for a proper interpretation of the outcomes of a study.

Processes, services and supply chain present different temporal characteristics which can lead to a distribution of emissions over very different time spans (days,years, decades or centuries). Also, the impact categories considered in LCA have specific temporal characteristics with different timescales. Various parameters used in conventional LCA present important temporal characteristics which are finally neglected.

As part of the DyPLCA project, this thesis work had for objective to contribute to the development of an operational method and tools for the time consideration in LCA. More precisely, models and software were developed for a dynamic approach of climate change and toxicity impact categories. This work contributed to the development of a temporal database and demonstrated the feasibility of coupling dynamic LCI and LCIA on an integrated framework.

The interest of the presented framework is to: 1) enable the practitioner of conventional LCA to use dynamic LCA without drastic changes with respect to the conventional method; 2) provide tools for both LCA steps and link them for a full dynamic LCA; and 3) present clear and comprehensible results without neglecting important temporal information.

At the level of the dynamic LCI, this work brought contribution for the development of a database with temporal parameters for processes and supply chains. This temporal database associated to ecoinvent v3.2 is necessary for building the network of processes and solving the dynamic LCI model for the background of any production system. This study contributed with data for chemical and biological processes presented in ecoinvent 3.2. Moreover, a deep analysis of ecoinvent processes allowed propositions for the improvement of the general dynamic LCI model. Several propositions have already been implemented in DyPLCA tool.

A dynamic approach was proposed for climate change impact category. Two indicators were proposed: radiative forcing (instantaneous and cumulated representing midpoint in the climate change cause-effect chain) and global mean temperature change. Both indicators have physical meaning and are involved in the cause-effect chain for the climate process. The impact results are obtained as values of indicators for any point in time. In the case of the mean temperature change, a maximum value is reached at some point in time depending on the GHG nature and emission profile. The proposed method is flexible in terms of time frame as it does not require a fixed time horizon, unlike the conventional LCA. The choice of an a priori time horizon is arbitrary as it does not reflect the temporal behaviour of the studied production system. The method does not use characterization factors. Instead, it calculates the impact indicators based on the real atmospheric burden determined by a given emission profile. Additionally, no reference substance is necessary. Another outcome of the dynamic approach is the possibility to account all types of carbon dioxide, i.e. fossil and biogenic. A sensitivity analysis performed on a case study demonstrated that the dynamic indicators are sensitive to the emission duration and position in time, but emission variations over short periods (less than one year) are not important for the impact results.

A dynamic approach for toxicity assessment was also proposed in this work. This model is based on the USEtox[®] framework and uses the Simplebox dynamic model for the substance fate calculation in function of time. Thus, the fate factor disappears and is replaced by the substance distribution in environmental compartments in function of time. Exposure and effect factors are unchanged and considered constant in time. Results for cancer human toxicity, non-cancer human toxicity and freshwater ecotoxicity are obtained. Characterization factors are no longer needed. Instead, two indicators are calculated: current toxicity in function of time as a measure of the instantaneous toxicity potential and cumulated toxicity in function of time as a measure of the total damage accounted at a given moment. Organic (non-persistent) and inorganic (persistent) substances have very different behaviours. Organic substances tend to be relatively rapidly removed from the environmental compartments and their fate follows similar evolution in time with the emission flow. Inorganic substances are mostly persistent and they accumulate in certain compartments; their toxicity potential lasts for centuries. These features are hidden in conventional LCA results. The sensitivity analysis conducted on a case study shown that the temporal definition of the LCI, i.e. the temporal characteristic of the substance emission (duration, variation in time, time granulometry), are determinant for the (eco)toxicity potential, especially for the human toxicity. Toxicity results are sensitive to time granulometry of 1 day, i.e. variations of emissions over one day are captured by the toxicity model and have repercussion on the impact results.

Finally, the complete framework was developed comprising the latest version of DyPLCA web application connected with the temporal database, the ecoinvent database and dynamic calculation of

impacts. The application in a case study demonstrates the functioning of the whole framework and the feasibility of a dynamic LCA.

The dynamic LCI tool provided a great coverage of the entire life cycle system and showed to be satisfactory when compared to the conventional inventory results (final mass balance of dynamic and conventional methods should be similar). Moreover, all emissions were correctly distributed over time according to the temporal parameters defined for the foreground processes and for the ones included in temporal database (for background processes). Regarding the dynamic LCIA step, the results obtained for climate change and toxicity impact categories showed the same features as those discussed in the dedicated chapters.

The presented dynamic LCA method is adapted for attributional type of evaluation. The technologies are considered unchanged over the time frame of the assessment, which could be quite large, e.g. 100 years. However this limitation occurs also in the attributional conventional LCA. Moreover, the adaptation of the described dynamic framework to the consequential type of evaluation was not yet investigated. For example, changes in the electricity mix in function of time are not considered in the background of dynamic inventory. Both ecoinvent and DyPLCA consider average values for the technology at a specific period of time and the characteristics of the electricity mix cannot be changed for the background. However, if the issue is important, the process (e.g. electricity mix) can be remodelled as foreground process. DyPLCA offers an appreciable capability of modelling a complex foreground system.

Concerning the impact models, some simplifying hypothesis could be alleviated in future developments. For example, the composition of the atmosphere is considered constant in time over the time span of the calculation, while the carbon dioxide concentration is expected to increase over decades. The same issue is encountered for toxicity model where all parameters are considered constant in time. However, modifications of the temperature for example lead to different parameter values.

Perspectives

Nevertheless, the development of a dynamic LCA method is still at the beginning. Further developments are crucial for the development of a fully operational method and tools, accepted and used by LCA practitioners. Several perspectives are mentioned in the following.

The methods implemented for the calculation of dynamic LCI and LCIA proved the feasibility of the temporal consideration in LCA. However, the computational time for case studies was important in both steps of LCA. *Optimizing the code* in order to decrease the computational time is necessary.

At this moment, even though the python models for dynamic LCIA are used with the output results of the DyPLCA tool for dynamic LCI, they are not part of the same IT platform. *The integration* of the LCIA model to the already existent web application would facilitate the use and would enable LCA practitioners to use more efficiently the developed framework without requiring the handling of different software for the calculation.

The model and related code implemented on DyPLCA tool should evolve by taking into account *specific behaviours of some process categories*, for example, processes needing a fixed date on calendar. This feature was already discussed in the project and needs a concrete implementation.

The case studies performed in this work concerned few technological fields (as foreground processes). Moreover, the aim of these case studies was mainly to evaluate the feasibility of the dynamic approach. Multiplying the *case studies in different areas* is necessary in order to evaluate more accurately the temporal characteristics of processes and supply chains. A case study in the construction field is currently being developed by CSTB - partner of the project. CSTB and LISBP are investigating dynamic aspects related to buildings construction and utilization.

The data used for the *development of the temporal database* took into account information from ecoinvent reports, other bibliography and assumptions. By this approach, generic data were attributed to process groups designated by ISIC. From now on, temporal data could be implemented by the contributors and developers of LCA databases which are in the best position to collect relevant information. Adding temporal characteristics in the temporal database would follow the same procedure as the input of material flow, environmental interventions, uncertainty, etc.

Considering the time dimension in LCIA, two impact categories were adapted for the dynamic method. In order to provide a broad range of possibilities in the *dynamic impact assessment*, more indicators have to be modelled by implementing the temporal dimension. Ozone depletion, terrestrial acidification and ionizing radiation are examples of impacts which have different temporal characteristics.

In the DyPLCA project, efforts were made for the use of models, methods and tools which are currently used in conventional LCA in order to have an easier adaptation and acceptability from LCA practitioners. Nevertheless, some outcomes are completely new and have to be interpreted differently than in conventional method. The *development of guidelines* for the use and interpretation of a dynamic LCA would be an important step for its acceptance by the LCA community.

This study aimed also at demonstrating the relevance of temporal consideration in LCA. In order to share and disseminate our findings, this work came out onto two peer-reviewed papers that were

already published and on one other submitted for publication. It was also communicated in three different conferences.

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Supplementary Information

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SI I Development of a temporal database for dynamic LCI

SI I.1 Liquid and gaseous fuels from biomass

Ecoinvent database presents 77 activities which are included in the ISIC group “Liquid and gaseous fuels from biomass”. This group was divided in two different parts for the designation of temporal parameters. It can be divided in products issued from fermentation reactions or products originated from chemical reactions.

Products from fermentation

The “Liquid and gaseous fuels from biomass” ISIC group presents datasets based on fermentation process (e.g. “ethanol production from wood” and ethanol production from potatoes “”). Fermentation processes have usually longer retention time than chemical processes in the reaction step which increases consequently the value of the parameter production period r .

The representative period T for the activities producing ethanol is based on the infrastructure activity “Ethanol fermentation plant” which has the lifetime of 20 years. Retention time in an ethanol production process is longer than for most of chemical processes. In the temporal database the production time parameter (r) was considered 3 days (Jungbluth et al., 2007).

In the case of the dataset “biogas production from grass” the data was retrieved in citation Jungbluth et al. (2007). Grass fermentation is considered a mesophilic reaction which, for processes such as fermentation of sewage sludge, manure and manure and biowaste, has a retention time in the fermenter between 28 and 30 days (Jungbluth et al., 2007). The retention time considered for the “biogas production from grass” activity was 30 days. The value of zero was attributed to delta, i.e. no storage between the biogas production and its use is considered.

Chemical products

Datasets such as “esterification of soybean oil” and “esterification of rape oil” have their production process mainly based on chemical reactions. For this reason, their temporal parameters were considered the same as the ones of “Manufacture of basic chemicals” ISIC group.

SI I.2 Manufacture of chemicals and chemical products

Ecoinvent database presents 34 activities which are included in the ISIC group “Manufacture of chemicals and chemical products”. This ISIC group is similar to the group “Manufacture of basic chemicals”. For this reason, the same temporal parameters were considered.

Exceptions

Activities which mention “...to generic market...” such as “1,1-dimethylcyclopentane to generic market for solvent, organic” and “fraction 1 from naphtha separation to generic market for chemical, organic” do not have the same temporal characteristics as the ISIC group “Manufacture of chemicals and chemical products” processes. Those activities have the purpose to link some processes to markets. There are no emissions or other activities presented in this dataset. Therefore, it is considered that the dataset does not have any temporal characteristics.

SI I.3 Manufacture of coke and refined petroleum products

Ecoinvent database presents 1 activity which is included in the ISIC group “Manufacture of coke and refined petroleum products”. This dataset represents the connection between a product and a market. Therefore, this activity does not present any temporal characteristics.

SI I.4 Manufacture of coke oven products

Ecoinvent database presents 5 activities which are included in the ISIC group “Manufacture of coke oven products”. The activity “hard coal coke factory” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period parameter T is based in the “hard coal coke factory” infrastructure activity. The value presented in this dataset is 30 years (Wernet et al., 2016). The value for the production period parameter r is considered 1 day.

SI I.5 Manufacture of fertilizers and nitrogen compounds

Ecoinvent database presents 72 activities which are included in the ISIC group “Manufacture of fertilizers and nitrogen compounds”. This group is similar to the group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

Activities that mention in the beginning of their name “Field application of...” are datasets that convert fertilisers in nitrogen or phosphorus equivalent. No temporal parameters were attributed to those datasets.

SI I.6 Manufacture of man-made fibres

Ecoinvent database presents 4 activities which are included in the ISIC group “Manufacture of man-made fibres”. The activity “pulp factory” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative parameter T is based in the “pulp factory” activity. The value presented in this dataset is 50 years (Hishier, 2007). The value for the parameter r is considered 1 day.

SI I.7 Manufacture of nuclear fuels

Ecoinvent database presents 74 activities which are included in the ISIC group “Manufacture of nuclear fuels”. The activity “nuclear fuel factory construction” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period parameter T is based in the “nuclear fuel factory construction” activity. The value presented in this dataset is 40 years (Dones et al., 2009). The value for the parameter r is considered 1 day.

SI I.8 Manufacture of other chemical products n.e.c.

Ecoinvent database presents 47 activities which are included in the ISIC group “Manufacture of other chemical products n.e.c.”. This group is similar to the group “Manufacture of basic chemicals”. For this reason, the same temporal parameters were considered.

Exceptions

The activity “blasting (blasting)” is considered as a service as it consists in the process of explosion of rocks. For this reason, r is considered 1 hour as it is a very fast process. The parameter δ is considered zero as there is no storage. The representative period parameter T of this activity is based in the lifetime of a mine which can be estimated as 20 years (Statista, 2015).

The activities “rosin size production, for paper production” and “Hydraulic fluid production, for geological stimulation” represent only the combination of different activities. No emission is linked to these datasets. It is considered that this activity does not present any temporal characteristics.

SI I.9 Manufacture of other rubber products

Ecoinvent database presents 3 activities which are included in the ISIC group “Manufacture of other rubber products”. The activity “tube insulation factory” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period parameter T is based in the “tube insulation factory” activity. The value presented in this dataset is 50 years (Kellenberger et al., 2007). The value for the production period parameter r is considered 1 day.

SI I.10 Manufacture of paints, varnishes and similar coatings, printing ink and mastics

Ecoinvent database presents 38 activities which are included in the ISIC group “Manufacture of paints, varnishes and similar coatings, printing ink and mastics”. This group is similar to the ISIC group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

SI I.11 Manufacture of pesticides and other agrochemical products

Ecoinvent database presents 147 activities which are included in the ISIC group “Manufacture of pesticides and other agrochemical products”. This group is similar to the ISIC group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

SI I.12 Manufacture of plastics and synthetic rubber in primary forms

Ecoinvent database presents 189 activities which are included in the ISIC group “Manufacture of plastics and synthetic rubber in primary forms”. This group is similar to the ISIC group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

SI I.13 Manufacture of plastics products

Ecoinvent database presents 86 activities which are included in the ISIC group “Manufacture of plastics products”. The activity “packaging box factory” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period T parameter is based in the “packaging box factory” activity. The value presented in this dataset is 50 years (Hishier, 2007). The value for the production period parameter r is considered 1 day.

Exception

The dataset “Collection of polystyrene scrap, post-consumer” does not contain any activity or emission. For this reason, it is considered that this activity does not present any temporal characteristics.

SI I.14 Manufacture of refined petroleum products

Ecoinvent database presents 143 activities which are included in the ISIC group “Manufacture of refined petroleum products”. The activity “petroleum refinery” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period T parameter is based in the “petroleum refinery” activity. The value presented in this dataset is 30 years (Wernet et al., 2016). The value for the production parameter r is considered 1 day.

Exceptions

Process that mention “import” in the name, such as “liquefied petroleum gas, import “ and light fuel oil, import from Europe “, works similarly to a market. Temporal characteristics are then neglected.

The activity “white spirit production (white spirit)” is similar to the activities presented into the group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

SI I.15 Manufacture of soap and detergents, cleaning and polishing preparations, perfumes and toilet preparations

Ecoinvent database presents 69 activities which are included in the ISIC group “Manufacture of soap and detergents, cleaning and polishing preparations, perfumes and toilet preparations”. This group is similar to the group “Manufacture of basic chemicals”. For this reason, same temporal parameters were here considered.

SI I.16 Sewerage

Ecoinvent database presents 95 activities which are included in the ISIC group “Sewerage”. The activity “wastewater treatment facility construction, capacity 1.6E8l/year” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period parameter T is based in the “wastewater treatment facility construction, capacity 1.6E8l/year” activity. The value presented in this dataset is 30 years (Doka, 2009). The value for the production period parameter r is considered 1 day. Others capacities are available in the report and with different lifetime.

SI I.17 Smelting and refining of uranium

Ecoinvent database presents 3 activities which are included in the ISIC group “Smelting and refining of uranium”. The activity “uranium conversion facility construction” is the infrastructure process which is present in most of the datasets in this ISIC group. For this reason, the representative period parameter T is based in the “uranium conversion facility construction” activity. The value presented in this dataset is 40 years (Wernet et al. 2016). The value for the production period parameter r is considered 1 day.

SI I.18 Water collection, treatment and supply

Ecoinvent database presents 60 activities which are included in the ISIC group “Water collection, treatment and supply”. The temporal data this group was based in the data presented for the

infrastructure activity “water works, capacity 1.1E10l/year”. The lifetime (representative period parameter T) considered in this activity is 60 years and production period parameter r is considered 1 day (Wernet et al., 2016).

Exceptions

Some processes have different characteristics and they were considered as exceptions. Hereafter, three exceptions are described: activities which mention “tap water production, seawater reverse osmosis, conventional pretreatment...”, activities of infrastructure and the activity “water, deionised, from tap water, at user”. The temporal parameters which are not cited in the paragraph are then the same as the ISIC group.

The process “tap water production, seawater reverse osmosis, conventional pre-treatment...” has a different production capacity as the one considered for the ISIC group. Therefore, the temporal characteristics of the activity “water works, capacity 6.23E10l/year” were considered for this process. The representative period parameter (T) of this process is 30 year (Wernet et al., 2016).

Activities of infrastructure production such as “ultrafiltration module production, hollow fiber” and “ultraviolet lamp production, for water disinfection” are treated as exceptions. The temporal parameters for this process were based in the data found in “Manufacture of basic chemicals”.

Finally, the process “water, deionised, from tap water, at user” is based in a different infrastructure dataset called “ion-exchanger production for water treatment “. This infrastructure presents a representative period of 15 year (Althaus et al., 2007).

SI II Temporal consideration in climate change impact assessment method**SI II.1 Parameters for the calculation of climate change impacts**

Table SI II.1 – Specific radiative forcing and lifetime for substances considered in climate change (IPCC, 2013)

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
(E)-1-Chloro-3,3,3-trifluoroprop-1-ene	4.00E-02	7.12E-02
(E)-HFC-1225ye	1.00E-02	1.34E-02
(E)-HFC-1234ze	4.00E-02	4.49E-02
(Trifluoromethyl) sulphur pentafluoride	5.90E-01	8.00E+02
(Z)-HFC-1225ye	2.00E-02	2.33E-02
(Z)-HFC-1234ze	2.00E-02	2.74E-02
(Z)-HFC-1336	7.00E-02	6.02E-02
1,1,1,2,2,3,3-Heptafluoro-3-(1,2,2,2-tetrafluoroethoxy)-propane	5.80E-01	6.70E+01
1,1,1,3,3,3-Hexafluoropropan-2-ol	2.60E-01	1.90E+00
1,1,1,3,3,3-Hexafluoropropan-2-yl formate	3.30E-01	3.20E+00
1,1,2,2-Tetrafluoro-1-(fluoromethoxy)ethane	3.40E-01	6.20E+00
1,1,2,2-Tetrafluoro-3-methoxy-propane	3.00E-02	3.89E-02
1,1,2-Trifluoro-2-(trifluoromethoxy)-ethane	3.50E-01	9.80E+00
1,1,3,3,4,4,6,6,7,7,9,9,10,10,12,12-hexadecafluoro-2,5,8,11-Tetraoxadodecane	1.43E+00	2.60E+01
1,1'-Oxybis[2-(difluoromethoxy)-1,1,2,2-tetrafluoroethane]	1.15E+00	2.60E+01
1,1-Difluoroethyl 2,2,2-trifluoroacetate	2.70E-01	3.00E-01
1,1-Difluoroethyl carbonofluoridate	1.70E-01	3.00E-01
1,2,2,2-Tetrafluoroethyl formate	3.50E-01	3.20E+00
1,2-Dichloroethane	1.00E-02	1.78E-01
1-Ethoxy-1,1,2,2,3,3,3-heptafluoropropane	2.80E-01	8.00E-01
1-Ethoxy-1,1,2,3,3,3-hexafluoropropane	1.90E-01	4.00E-01
2,2,2-Trifluoroethanol	1.00E-01	3.00E-01
2,2,2-Trifluoroethyl 2,2,2-trifluoroacetate	1.50E-01	1.50E-01
2,2,2-Trifluoroethyl formate	1.60E-01	4.00E-01
2,2,3,3,3-Pentafluoropropan-1-ol	1.40E-01	3.00E-01
2,2,3,3,4,4,4-Heptafluoro-1-butanol	1.60E-01	3.00E-01
2,2,3,3,4,4,4-Heptafluorobutan-1-ol	2.00E-01	6.00E-01
2,2,3,3,4,4,5,5-Octafluorocyclopentanol	1.60E-01	3.00E-01
2,2,3,3-Tetrafluoro-1-propanol	1.10E-01	2.50E-01
2,2,3,4,4,4-Hexafluoro-1-butanol	1.90E-01	2.60E-01
2,2-Difluoroethanol	4.00E-02	1.10E-01
2-Chloro-1,1,2-trifluoro-1-methoxyethane	2.10E-01	1.40E+00
2-Ethoxy-3,3,4,4,5-pentafluorotetrahydro-2,5-bis[1,2,2,2-	4.90E-01	1.00E+00

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
tetrafluoro-1-(trifluoromethyl)ethyl]-furan		
2-Fluoroethanol	2.00E-02	5.59E-02
3,3,3-Trifluoropropan-1-ol	2.00E-02	3.29E-02
3,3,3-Trifluoro-propanal	4.00E-03	5.48E-03
3,3,3-Trifluoropropyl formate	1.30E-01	3.00E-01
3,3,4,4,5,5,6,6,6-Nonafluorohex-1-ene	3.00E-02	2.08E-02
3,3,4,4,5,5,6,6,7,7,7-Undecafluoroheptan-1-ol	6.00E-02	5.48E-02
3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooct-1-ene	3.00E-02	2.08E-02
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-Hep- tadecafluorodec-1-ene	3.00E-02	2.08E-02
3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,11,11,11-Non- adecafluoroundecan-1-ol	5.00E-02	5.48E-02
3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-Pentadecafluorononan-1-ol	7.00E-02	5.48E-02
4,4,4-Trifluorobutan-1-ol	1.00E-02	1.10E-02
Carbon dioxide	1.37E-05	3.94E+02
Carbon tetrachloride	1.70E-01	2.60E+01
CFC-11	2.60E-01	4.50E+01
CFC-113	3.00E-01	8.50E+01
CFC-114	3.10E-01	1.90E+02
CFC-115	2.00E-01	1.02E+03
CFC-12	3.20E-01	1.00E+02
CFC-13	2.50E-01	6.40E+02
Chloroform	8.00E-02	4.00E-01
Difluoro(fluoromethoxy)methane	3.00E-01	3.30E+00
Difluoro(methoxy)methane	1.70E-01	1.10E+00
Difluoromethyl 2,2,2-trifluoroacetate	2.40E-01	3.00E-01
Ethyl 2,2,2-trifluoroacetate	5.00E-02	6.00E-02
Fluoro(fluoromethoxy)methane	1.90E-01	9.00E-01
Fluoro(methoxy)methane	7.00E-02	2.00E-01
Fluoroxene	1.00E-02	9.86E-03
Halon-1201	1.50E-01	5.20E+00
Halon-1202	2.70E-01	2.90E+00
Halon-1211	2.90E-01	1.60E+01
Halon-1301	3.00E-01	6.50E+01
Halon-2301	1.40E-01	3.40E+00
Halon-2311 / Halothane	1.30E-01	1.00E+00
Halon-2401	1.90E-01	2.90E+00
Halon-2402	3.10E-01	2.00E+01
HCFC-122	1.70E-01	1.00E+00
HCFC-122a	2.10E-01	3.40E+00
HCFC-123	1.50E-01	1.30E+00
HCFC-123a	2.30E-01	4.00E+00

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
HCFC-124	2.00E-01	5.90E+00
HCFC-132c	1.70E-01	4.30E+00
HCFC-141b	1.60E-01	9.20E+00
HCFC-142b	1.90E-01	1.72E+01
HCFC-21	1.50E-01	1.70E+00
HCFC-22	2.10E-01	1.19E+01
HCFC-225ca	2.20E-01	1.90E+00
HCFC-225cb	2.90E-01	5.90E+00
HCFE-235ca2 (enflurane)	4.10E-01	4.30E+00
HCFE-235da2 (isoflurane)	4.20E-01	3.50E+00
HFC-1132a	4.00E-03	1.10E-02
HFC-1141	2.00E-03	5.75E-03
HFC-1234yf	2.00E-02	2.87E-02
HFC-1243zf	1.00E-02	1.92E-02
HFC-125	2.30E-01	2.82E+01
HFC-134	1.90E-01	9.70E+00
HFC-1345zfc	1.00E-02	2.08E-02
HFC-134a	1.60E-01	1.34E+01
HFC-143	1.30E-01	3.50E+00
HFC-143a	1.60E-01	4.71E+01
HFC-152	4.00E-02	4.00E-01
HFC-152a	1.00E-01	1.50E+00
HFC-161	2.00E-02	1.81E-01
HFC-227ca	2.70E-01	2.82E+01
HFC-227ea	2.60E-01	3.89E+01
HFC-23	1.80E-01	2.22E+02
HFC-236cb	2.30E-01	1.31E+01
HFC-236ea	3.00E-01	1.10E+01
HFC-236fa	2.40E-01	2.42E+02
HFC-245ca	2.40E-01	6.50E+00
HFC-245cb	2.40E-01	4.71E+01
HFC-245ea	1.60E-01	3.20E+00
HFC-245eb	2.00E-01	3.10E+00
HFC-245fa	2.40E-01	7.70E+00
HFC-263fb	1.00E-01	1.20E+00
HFC-272ca	7.00E-02	2.60E+00
HFC-32	1.10E-01	5.20E+00
HFC-329p	3.10E-01	2.84E+01
HFC-365mfc	2.20E-01	8.70E+00
HFC-41	2.00E-02	2.80E+00
HFC-43-10mee	4.20E-01	1.61E+01
HFE-125	4.10E-01	1.19E+02

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
HFE-134 (HG-00)	4.40E-01	2.44E+01
HFE-143a	1.80E-01	4.80E+00
HFE-216	2.00E-02	2.30E-02
HFE-227ea	4.40E-01	5.16E+01
HFE-236ca	5.60E-01	2.08E+01
HFE-236ca12 (HG-10)	6.50E-01	2.50E+01
HFE-236ea2 (desflurane)	4.50E-01	1.08E+01
HFE-236fa	3.60E-01	7.50E+00
HFE-245cb2	3.30E-01	4.90E+00
HFE-245fa1	3.10E-01	6.60E+00
HFE-245fa2	3.60E-01	5.50E+00
HFE-254cb1	2.60E-01	2.50E+00
HFE-263fb2	4.00E-02	6.30E-02
HFE-263m1	1.30E-01	4.00E-01
HFE-329mcc2	5.30E-01	2.25E+01
HFE-329me3	4.80E-01	4.00E+01
HFE-338mcf2	4.40E-01	7.50E+00
HFE-338mmz1	4.40E-01	2.12E+01
HFE-338pcc13 (HG-01)	8.60E-01	1.29E+01
HFE-347mcc3 (HFE-7000)	3.50E-01	5.00E+00
HFE-347mcf2	4.20E-01	6.60E+00
HFE-347mmy1	3.20E-01	3.70E+00
HFE-347pcf2	4.80E-01	6.00E+00
HFE-356mec3	3.00E-01	3.80E+00
HFE-356mff2	1.70E-01	2.87E-01
HFE-356mmz1	1.50E-01	2.66E-01
HFE-356pcc3	3.20E-01	3.80E+00
HFE-356pcf2	3.70E-01	5.70E+00
HFE-356pcf3	3.80E-01	3.50E+00
HFE-365mcf2	2.60E-01	6.00E-01
HFE-365mcf3	5.00E-02	5.28E-02
HFE-374pc2	3.00E-01	5.00E+00
HFE-43-10pccc124 (H-Galden 1040x, HG-11)	1.02E+00	1.35E+01
HFE-449s1 (HFE-7100)	3.60E-01	4.70E+00
HFE-569sf2 (HFE-7200)	3.00E-01	8.00E-01
HG-02	1.24E+00	1.29E+01
HG-03	1.76E+00	1.29E+01
HG-20	9.20E-01	2.50E+01
HG-21	1.71E+00	1.35E+01
HG-30	1.65E+00	2.50E+01
HG'-01	2.90E-01	2.00E+00
HG'-02	5.60E-01	2.00E+00

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
HG ¹ -03	7.60E-01	2.00E+00
i-HFE-7100	3.50E-01	4.70E+00
i-HFE-7200	2.40E-01	8.00E-01
Methane	3.63E-04	1.24E+01
Methyl 2,2,2-trifluoroacetate	1.80E-01	6.00E-01
Methyl 2,2-difluoroacetate	5.00E-02	1.10E-01
Methyl bromide	4.00E-03	8.00E-01
Methyl carbonofluoridate	7.00E-02	1.80E+00
Methyl chloride	1.00E-02	1.00E+00
Methyl chloroform	7.00E-02	5.00E+00
Methylene bromide	1.00E-02	3.00E-01
Methylene chloride	3.00E-02	4.00E-01
n-HFE-7100	4.20E-01	4.70E+00
n-HFE-7200	3.50E-01	8.00E-01
Nitrogen trifluoride	2.00E-01	5.00E+02
Nitrous Oxide	3.00E-03	1.21E+02
perfluoro-2-methyl-3-pentanone	3.00E-02	1.92E-02
Perfluorobut-1-ene	2.00E-02	1.64E-02
Perfluorobut-2-ene	7.00E-02	8.49E-02
Perfluorobuta-1,3-diene	3.00E-03	3.01E-03
Perfluorobutyl acetate	1.20E-01	6.00E-02
Perfluorobutyl formate	5.60E-01	3.00E+00
Perfluorocyclopentene	8.00E-02	8.49E-02
Perfluorodecalin (cis)	5.60E-01	2.00E+03
Perfluorodecalin (trans)	4.80E-01	2.00E+03
Perfluoroethyl acetate	1.00E-01	6.00E-02
Perfluoroethyl formate	4.40E-01	3.50E+00
Perfluoropropyl acetate	1.10E-01	6.00E-02
Perfluoropropyl formate	5.00E-01	2.60E+00
PFC-1114	2.00E-03	3.01E-03
PFC-116	2.50E-01	1.00E+04
PFC-1216	1.00E-02	1.34E-02
PFC-14	9.00E-02	5.00E+04
PFC-218	2.80E-01	2.60E+03
PFC-31-10	3.60E-01	2.60E+03
PFC-41-12	4.10E-01	4.10E+03
PFC-51-14	4.40E-01	3.10E+03
PFC-61-16	5.00E-01	3.00E+03
PFC-71-18	5.50E-01	3.00E+03
PFC-91-18	5.50E-01	2.00E+03
PFC-c216	2.30E-01	3.00E+03
PFPME (perfluoropolymethylisopropyl ether)	6.50E-01	8.00E+02

Compound	Specific radiative forcing ($\text{W}\cdot\text{m}^{-2}\cdot\text{ppb}^{-1}$)	Lifetime (years)
Sevoflurane (HFE-347mmz1)	3.20E-01	2.20E+00
Sulphur hexafluoride	5.70E-01	3.20E+03
Sulphuryl fluoride	2.00E-01	3.60E+01
Trifluoro(fluoromethoxy)methane	3.30E-01	4.40E+00
Trifluoromethyl formate	3.10E-01	3.50E+00

Table SI II.2 - Estimates of the parameters in IRF CO_2 (Joos et al., 2013).

τ_1 (year)	394.4
τ_2 (year)	36.54
τ_3 (year)	4.3
a_0	0.217
a_1	0.224
a_2	0.282
a_3	0.276

Table SI II.3- Parameters for the temperature impulse response function IRF_T (Boucher and Reddy, 2008)

f_1 ($\text{K}\cdot\text{m}^2\cdot\text{W}^{-1}$)	0.631
f_2 ($\text{K}\cdot\text{m}^2\cdot\text{W}^{-1}$)	0.429
d_1	8.4
d_2	409.5

SI III Environmental assessment of bioenergy production from microalgae based systems

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SI III.1 Parameters and energetic data for processes.

Table SI III.1 – Parameters and energetic data for processes.

	Value	Unit	Reference	Microalgae
Culture				
Production rate	30	$\text{g m}^{-2} \text{d}^{-1}$	Borowitzka, 1990	<i>Dunalliella salina</i>
Doubling	12	h	Borowitzka, 1990	<i>Dunalliella salina</i>
Microalgae formula	$\text{CH}_{1.83}\text{O}_{0.48}$ $\text{N}_{0.11}\text{P}_{0.01}$		Chisti, 2007	General Formula
Microalgae composition	Ash: $9\pm 1\%$		Renaud et al., 1994	<i>Dunalliella salina</i>
	Protein: $40.3\pm 2.8\%$			
	Carbohydrate: $1.0\pm 1\%$			
	Lipid: $28.1\pm 1.2\%$			
	chlorophyll a: $1.26\pm 0.1\%$			
Flue gas composition	NO: 0.015%		Brown, 1996	-
	SO ₂ : 0.02%			
	O ₂ : 5%			
	CO ₂ : 13.6%			
	N ₂ : 81.365%			
Electricity	0.227	kWh/kg dry MA culture	Kadam, 2001	Generic model
Nitrogen fertiliser	0.188	kg Ammonium Nitrate/ kg dry MA culture	Calculation	-
Potassium fertiliser	0.144	kg Single Superphosphate/kg dry MA culture	Calculation	-
Electricity	1.332	kWh/kg dry harvested MA	Watropur, 2015	Process specification
Flocculation				
Soda (0.01 mol/L)	0.9	kg/kg dry harvested MA	Besson & Guiraud, 2013	<i>Dunalliella salina</i>
Electricity	0.41	kWh/kg dry harvested MA	Ecologix environmental systems, 2015	Machine specification
Factor of concentration	20		Besson & Guiraud, 2013	<i>Dunalliella salina</i>
Dewatering				
Electricity	0.069	kWh/kg dry harvested MA	PWTech, 2015	Process specification

Drying				
Electricity	1.332	kWh/kg dry harvested MA	Watropur, 2015	Process specification
Supercritical Extraction				
CO ₂ rate	0.6	kg/h per	Nikitine et al., 2009	Not specified
Pressure	30	MPa	Nikitine et al., 2009	Not specified
Temperature	323	K	Nikitine et al., 2009	Not specified
Electricity	3.5	kWh/kg oil	Calculation	-
Heat	46	MJ/ kg oil	Calculation	-
Make up CO ₂	10	% of feed	Perrut, 2000	Process specification
Supercritical Transesterification				
Methanol	1.668	kg MeOH/ kg biodiesel	Saka & Kusdiana, 2000	-
Pressure	19	MPa	Saka & Kusdiana, 2000	-
Temperature	623	K	Saka & Kusdiana, 2000	-
Electricity	0.0089	kWh/kg biodiesel	Calculation	-
Heat	2.4	MJ/ kg biodiesel	Calculation	-
Purification				
Heat	1.24	MJ/ kg biodiesel	Glisic & Skala, 2009	-
Digestion				
Digestion concentration	7	%	Ehimen et al. 2009	<i>Chlorella sp</i>
Electricity Consumption	0.734	kWh/ kg CH ₄	Collet et al., 2011	<i>Chlorella vulgaris</i>
Heat Consumption	13.482	MJ/ kg CH ₄	Collet et al., 2011	<i>Chlorella vulgaris</i>
Electricity Production	17.76	kWh/ kg CH ₄	Ecoinvent v2.2 Database	-
Heat Production	30.525	MJ/ kg CH ₄	Ecoinvent v2.2 Database	-

SI III.2 Data for infrastructure.

Table SI III.2 – BD Infrastructure data for a 100 ha plant of biomass production.

	Value	Unit	Reference
Culture pond			
Concrete	109167	m ³	Lardon et al., 2009
PVC	1200000	kg	
Steel	70000	kg	
Glass fibre	256000	kg	
Dewatering			
Steel	31200	kg	PWTech, 2015
Drying			
Steel	224600	kg	Watropur, 2015
Supercritical extraction			
Steel	5192	kg	Separex, 2015
Supercritical transesterification			
Steel	20838	kg	Separex, 2015
Purification			
Steel	6688	kg	Glisic and Skala, 2009
Digestion			
Concrete	902.9	kg	Collet et al. 2011

Table SI III.3 – BG Infrastructure data for a 100 ha plant of biomass production.

	Value	Unit	Reference
Culture pond			
Concrete	109167	m ³	Lardon et al., 2009
PVC	1200000	kg	
Steel	70000	kg	
Glass fibre	256000	kg	
Dewatering			
Steel	31200	kg	PWTech, 2015
Digestion			
Concrete	902.9	kg	Collet et al. 2011

SI III.3 Data for life cycle inventory

Table SI III.4 – Inventory for the production of 1 MJ of biodiesel.

Process	Operational data	Ecoinvent process	Unit	Value
Culture	infrastructure	polyvinylchloride, at regional storage [RER]	kg	5.47x10 ⁻⁴
		steel, low-alloyed, at plant [RER]	kg	3.19x10 ⁻⁵
		glass fibre, at plant [RER]	kg	1.17x10 ⁻⁴
		concrete, normal, at plant [CH]	m ³	8.55x10 ⁻⁵
	electricity	electricity mix [FR]	kWh	2.73x10 ⁻²
	fertilisers	single superphosphate, as P ₂ O ₅ , at regional storage [RER]	kg	1.26x10 ⁻³
		ammonium nitrate, as N, at regional storehouse [RER]	kg	3.95x10 ⁻³
	transport	transport, barge [RER]	tkm	4.07x10 ⁻³
		transport, freight, rail [FR]	tkm	5.21x10 ⁻⁴
		transport, lorry 20-28t, fleet average [CH]	tkm	5.21x10 ⁻⁴
emission	carbon dioxide, fossil [air/ high population]	kg	1.12x10 ⁻²	
Flocculation	electricity	electricity mix [FR]	kWh	4.45x10 ⁻²
	chemical	sodium hydroxide, 50% in H ₂ O, production mix, at plant [RER]	kg	8.66x10 ⁻⁵
	transport	transport, lorry 20-28t, fleet average [CH]	tkm	1.73x10 ⁻⁶
Dewatering	electricity	electricity mix [FR]	kWh	7.49x10 ⁻⁴
	infrastructure	steel, low-alloyed, at plant [RER]	kg	1.42x10 ⁻⁵
Dryer	electricity	electricity mix [FR]	kWh	1.44x10 ⁻¹
	infrastructure	steel, low-alloyed, at plant [RER]	kg	1.02x10 ⁻⁴
Extraction	transport	transport, lorry 20-28t, fleet average [CH]	tkm	2.17x10 ⁻⁴
	chemical	liquid carbon dioxide, at plant [RER]	kg	1.08x10 ⁻²
	infrastructure	steel, low-alloyed, at plant [RER]	kg	2.37x10 ⁻⁶
	electricity	electricity mix [FR]	kWh	1.26x10 ⁻¹
	heat	heat, natural gas, at industrial furnace > 100 kW [RER]	MJ	7.69x10 ⁻¹
Transesterification	infrastructure	steel, low-alloyed, at plant [RER]	kg	9.51x10 ⁻⁶
	chemical	methanol, at plant [GLO]	kg	3.07x10 ⁻³
	transport	transport, lorry 20-28t, fleet average [CH]	tkm	9.21x10 ⁻⁴
		transport, barge [RER]	tkm	1.38x10 ⁻²
	electricity	electricity mix [FR]	kWh	8.00x10 ⁻⁴
	heat	heat, natural gas, at industrial furnace > 100 kW [RER]	MJ	6.45x10 ⁻²
Purification	infrastructure	steel, low-alloyed, at plant [RER]	kg	3.05x10 ⁻⁶
	transport	transport, lorry 20-28t, fleet average [CH]	tkm	5.29x10 ⁻²
	heat	heat, natural gas, at industrial furnace > 100 kW [RER]	MJ	3.29x10 ⁻²
Combustion	product	Energy from combustion	MJ	1
	emission	carbon dioxide, fossil [air/ high population]	kg	4.41x10 ⁻²
Anaerobic	infrastructure	concrete, normal, at plant [CH]	m ³	5.97x10 ⁻⁷

Process	Operational data	Ecoinvent process	Unit	Value	
digestion	electricity	electricity mix [FR]	kWh	1.08x10 ⁻²	
	heat	heat, natural gas, at industrial furnace > 100 kW [RER]	MJ	1.98x10 ⁻¹	
Cogeneration	infrastructure	cogen unit 160 kWe, common components for heat+electricity	unit	4.07x10 ⁻⁹	
	maintenance	lubrication oil, at plant [RER]	kg	2.44x10 ⁻⁵	
	disposal	disposal, used mineral oil, 10% water, to hazardous waste incineration [CH]	kg	2.44x10 ⁻⁵	
	emissions		Heat, waste [air/unspecified]	kg	1.06x10 ⁻¹
			Nitrogen oxides [air/low population density]	kg	1.22x10 ⁻⁵
			Carbon monoxide, biogenic [air/low population density]	kg	3.91x10 ⁻⁵
			carbon dioxide, biogenic [air/low population density]	kg	6.78x10 ⁻²
			methane, biogenic [air/low population density]	kg	1.87x10 ⁻⁵
			NMVOC, non-methane volatile organic compounds, unspecified origin [air/low population density]	kg	1.63x10 ⁻⁶
			Dinitrogen monoxide [air/low population density]	kg	2.04x10 ⁻⁶
			Sulfur dioxide [air/low population density]	kg	1.71x10 ⁻⁵
			Platinum [air/low population density]	kg	5.70x10 ⁻¹²
		carbon dioxide, fossil [air/ high population]	kg	3.77x10 ⁻²	
	product	Heat production	MJ	4.48x10 ⁻¹	
product	Electricity production	kWh	7.24x10 ⁻²		
Spreading	emissions	Dinitrogen monoxide [air/high population density]	kg	2.00x10 ⁻⁴	
		Ammonia [air/high population density]	kg	2.10x10 ⁻³	
		Phosphate [water/ground-]	kg	7.90x10 ⁻⁶	
		Phosphate [water/river]	kg	2.78x10 ⁻⁵	
	service	slurry spreading, by vacuum tanker [CH]	m ³	1.15x10 ⁻⁴	

Table SI III.5 – Inventory for the production of 1 MJ of biogas

Process	Operational data	Ecoinvent process	Unit	Value
Culture	infrastructure	polyvinylchloride, at regional storage [RER]	kg	3.05x10 ⁻⁷
		steel, low-alloyed, at plant [RER]	kg	2.29x10 ⁻⁸
		glass fibre, at plant [RER]	kg	6.52x10 ⁻⁸
		concrete, normal, at plant [CH]	m ³	3.04x10 ⁻⁸
	electricity	electricity mix [FR]	kWh	1.53x10 ⁻²
	fertilisers	single superphosphate, as P ₂ O ₅ , at regional storage [RER]	kg	7.04x10 ⁻⁴
		ammonium nitrate, as N, at regional storehouse [RER]	kg	2.21x10 ⁻⁴
	transport	transport, barge [RER]	tkm	4.81x10 ⁻⁴

Process	Operational data	Ecoinvent process	Unit	Value
		transport, freight, rail [FR]	tkm	9.25x10 ⁻⁵
		transport, lorry 20-28t, fleet average [CH]	tkm	9.25x10 ⁻⁵
	emission	carbon dioxide, fossil [air/ high population]	kg	6.63x10 ⁻³
Flocculation	electricity	electricity mix [FR]	kWh	2.48x10 ⁻²
	chemical	sodium hydroxide, 50% in H ₂ O, production mix, at plant [RER]	kg	4.83x10 ⁻⁵
	transport	transport, lorry 20-28t, fleet average [CH]	tkm	9.67x10 ⁻⁷
Dewatering	electricity	electricity mix [FR]	kWh	3.76x10 ⁻⁴
	infrastructure	steel, low-alloyed, at plant [RER]	kg	7.15x10 ⁻⁶
Anaerobic digestion	infrastructure	concrete, normal, at plant [CH]	m ³	4.60x10 ⁻⁷
	electricity	electricity mix [FR]	kWh	1.16x10 ⁻³
	heat	heat, natural gas, at industrial furnace > 100 kW [RER]	MJ	2.64x10 ⁻²
Cogeneration	infrastructure	cogen unit 160 kWe, common components for heat+electricity	unit	5.00x10 ⁻⁹
	maintenance	lubrication oil, at plant [RER]	kg	3.00x10 ⁻⁵
	disposal	disposal, used mineral oil, 10% water, to hazardous waste incineration [CH]	kg	3.00x10 ⁻⁵
	emissions	Heat, waste [air/unspecified]	kg	1.30x10 ⁻⁴
		Nitrogen oxides [air/low population density]	kg	1.50x10 ⁻⁵
		Carbon monoxide, biogenic [air/low population density]	kg	4.80x10 ⁻⁵
		carbon dioxide, biogenic [air/low population density]	kg	8.33x10 ⁻²
		methane, biogenic [air/low population density]	kg	2.30x10 ⁻⁵
		NM VOC, non-methane volatile organic compounds, unspecified origin [air/low population density]	kg	2.00x10 ⁻⁶
		Dinitrogen monoxide [air/low population density]	kg	2.50x10 ⁻⁶
		Sulfur dioxide [air/low population density]	kg	2.10x10 ⁻⁵
		Platinum [air/low population density]	kg	7.00x10 ⁻¹²
		carbon dioxide, fossil [air/ high population]	kg	2.70x10 ⁻²
		Heat production	MJ	5.5x10 ⁻¹
	Electricity production	kWh	8.89x10 ⁻²	
Spreading	emissions	Dinitrogen monoxide [air/high population density]	kg	1.85x10 ⁻⁵
		Ammonia [air/high population density]	kg	3.04x10 ⁻⁴
		Phosphate [water/ground-]	kg	4.57x10 ⁻⁶
		Phosphate [water/river]	kg	1.61x10 ⁻⁵
	service	slurry spreading, by vacuum tanker [CH]	m ³	8.34x10 ⁻⁴

SI III.4 Calculation of fertilisers

A general microalgae formula (equation SI III.1) found in Grobeelar (2007 as cited in Chisti, 2007) was used for the calculation of fertiliser requirements:



From SI III.1, microalgae molecular mass was calculated as 2.34×10^1 g/mol.

In this sense, the nutriment for the culture of 1 kg of microalgae can be calculated as follows:

$$C = 5.14 \times 10^{-1} \text{ kg};$$

$$N = 6.597 \times 10^{-2} \text{ kg};$$

$$H = 7.90 \times 10^{-2} \text{ kg};$$

$$O = 3.28 \times 10^{-1} \text{ kg};$$

$$P = 1.32 \times 10^{-2} \text{ kg}$$

In the database used for life cycle inventory calculation (Ecoinvent v2.2 in Frischknecht et al. 2005), ammonium nitrate was chosen as nitrogen source and this substance is counted in N [kg] basis in the database. Also, single superphosphate was chosen and phosphorus source and the substance is counted in P_2O_5 [kg] basis in the database.

When calculating the need of ammonium nitrate as N [kg], we obtain 0.0660 kg of N required per kg of microalgae produced which was equivalent to 0.188 kg of ammonium nitrate per kg of biomass produced.

When calculating the need of phosphate fertiliser (single superphosphate) as P, we obtain 0.0132 kg of P required per kg of microalgae produced. Then, we obtain 0.0302 kg of P_2O_5 required per kg of biomass produced which was equivalent to 0.144 kg of single superphosphate per kg of biomass produced.

SI III.5 Calculation of super critical extraction and super critical transesterification

In experiments conducted for supercritical processes, to reach supercritical parameters, the solvent passed first through a pump where pressure is increased to the supercritical pressure and then by a heat exchanger where the solvent temperature is increased to reach the supercritical temperature. Finally, extraction or transesterification are performed. (Mendes et al., 1994; Bunyakiat et al., 2006). Data for energy consumption in the supercritical processes were not provided by the authors. In this sense, for this work the energy required for pumping step was calculated and also energy required for heating was calculated by means of thermodynamic curves.

Regarding the calculation of the energy required in the pumping step, we can use Bernoulli's equation to calculate the energy of the pump by a unit of mass w_p (J/kg):

$$P_{out}/\rho + V_{out}^2/2 + gz_{out} = P_{in}/\rho + V_{in}^2/2 + gz_{in} - loss + w_p \quad (\text{SI III.2})$$

Where P is pressure, V is the velocity of the fluid, z is the elevation, ρ represents the density of the fluid, g is the gravity and loss stands for the loss of charge per unit of mass.

Considering that there are no charge losses and there are no changes in fluid velocity and elevation, equation SI III.2 becomes SI III.3:

$$w_p = (P_{out} - P_{in})/\rho \quad (\text{SI III.3})$$

As w_p is the energy required by unit of mass (SI III.4), the total energy (E) necessary for pumping is represented by SI III.5.

$$w_p = E/m \quad (\text{SI III.4})$$

$$E = m_{solvent} \Delta P / \rho_{solvent} \quad (\text{SI III.5})$$

Where E is energy requirement and m is the mass of solvent.

Considering that the efficiency of the pump is 80%, equation SI III.4 becomes:

$$E = m_{solvent} \Delta P / 0.8 \rho_{solvent} \quad (\text{SI III.6})$$

Equation SI III.7 results in the energy for pumping CO₂ in the supercritical extraction step.

$$E \text{ (MJ/kg of oil)} = \left(\frac{m_{CO_2}}{m_{oil}} \right) \frac{\Delta P * 10^{-6}}{0.8 \rho_{CO_2}} \quad (\text{SI III.7})$$

Equation SI III.8 shows the energy for pumping methanol in the supercritical transesterification step.

$$E \text{ (MJ/kg of biodiesel)} = \left(\frac{m_{MeOH}}{m_{biodiesel}} \right) \frac{\Delta P * 10^{-6}}{0.8 \rho_{MeOH}} \quad (\text{SI III.8})$$

In supercritical extraction, the input conditions for the pump were: pressure of 0.1 MPa and temperature of 285.15K. Output conditions were: pressure of 30MPa and temperature of 285.15K). In supercritical transesterification, the input conditions for the pump were: pressure of 0.1 MPa and temperature of 293.15K. Output conditions were: pressure of 19MPa and temperature of 293.15K).

For the calculation of heat requirements, a graphic between enthalpy (kJ/kg) and Temperature (K) was generated (graphics were generated in Linstrom and Mallard ,2015) in isobaric conditions in order to calculate the energy necessary for heating the input solvents in the supercritical processes.

In supercritical extraction, the input conditions for the heat exchanger were: pressure of 30MPa and temperature of 285.15K. Output conditions were: pressure of 30MPa and temperature of 335.15K). Pressure drop in heat exchanger was neglected.

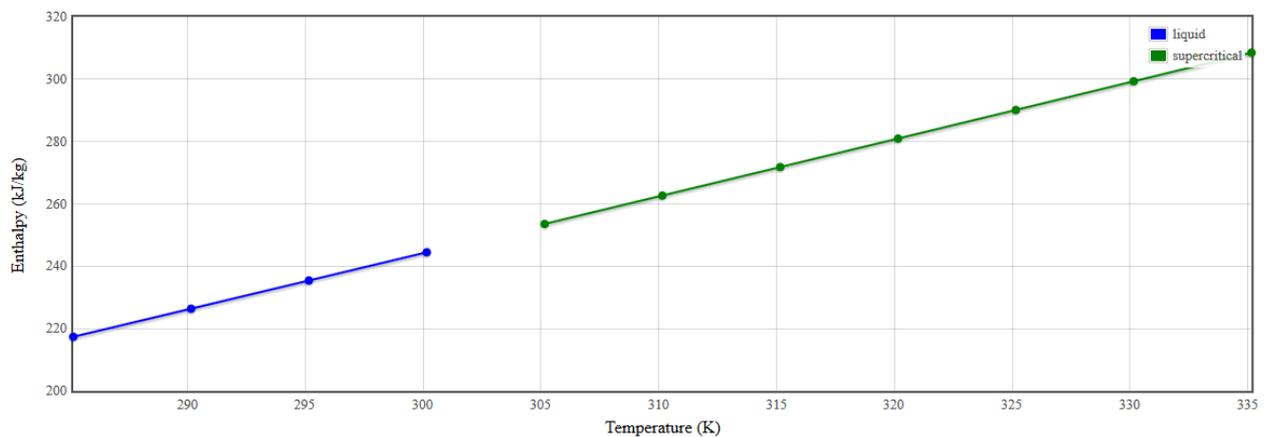


Figure SI III.1 – Carbon dioxide isobaric enthalpy curve at 30MPa for temperatures between 285.15K and 335.15K [H_1 (285.15 K, 15° C) is 217 kJ/kg of solvent CO_2 and H_2 (335.15 K, 60°C) is 309 kJ/kg of solvent CO_2].

The energy necessary for heating in the extraction step can be calculated using the results obtained in the graphic (Figure SI III.1) and using equation SI III.9.

$$E_{heating} (MJ/kg \text{ of oil}) = (H_2 - H_1) * (\text{mass of } CO_2 / \text{mass of extracted oil}) * 10^{-3} \text{ (SI III.9)}$$

In supercritical transesterification, the input conditions for the heat exchanger were: pressure of 19MPa and temperature of 293.15K. Output conditions were: pressure of 19MPa and temperature of 613.15K. Pressure drop in heat exchanger was neglected.

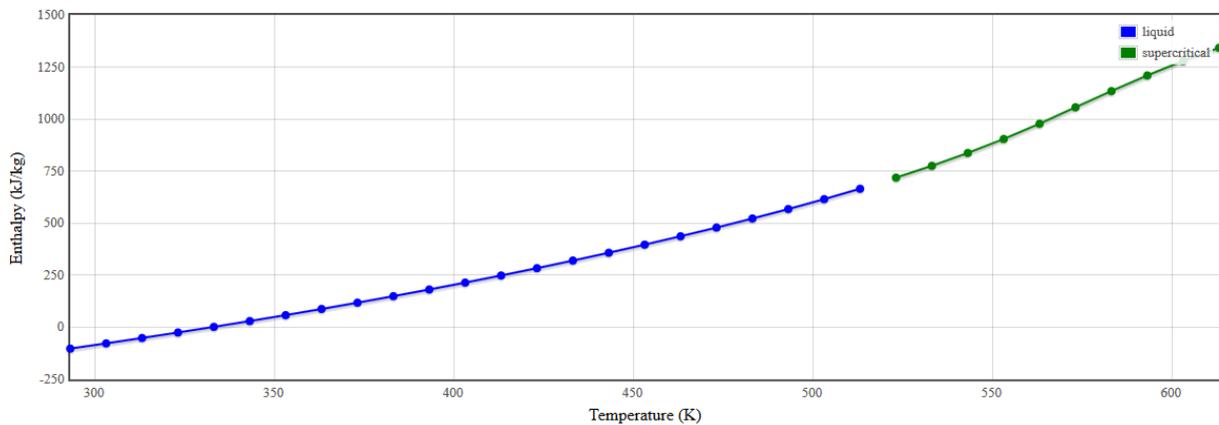


Figure SI III.2 – Methanol isobaric enthalpy curve at 19MPa for temperatures between 293.15K and 613.15K (H_1 (293.15, 25°C): -102.20 kJ/kg of methanol and H_2 (613.15, 340°C):1342.8 kJ/kg of methanol)

The energy necessary for heating in the extraction step can be calculated using the results obtained in the graphic (Figure SI III.2) and using equation SI III.10.

$$E_{heating} (MJ/kg \text{ of biodiesel}) = (H_2 - H_1) * (\text{mass of } CO_2 / \text{mass of biodiesel}) * 10^{-3} \text{ (SI III.10)}$$

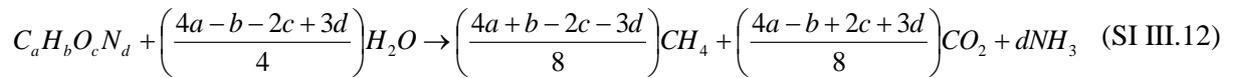
The results for energy requirements in supercritical processes can be found in SI III.1.

SI III.6 Biogas production

The microalgae formula (SI III.1) was used to calculate the formula of the biomass entering the digestion step. In the biodiesel process, lipid content, which composition can be seen in equation SI III.11, should be extracted from microalgae formula.



Sialve et al. (SI III.12) show the equation which considers the maximum efficiency for biogas production:



Considering 75% of efficiency in biogas production, the resulting quantities of biogas could be calculated and the results for biogas can be found in SI III.1.

SI III.7 Climate parameters for CO₂, CH₄ and N₂OTable SI III.6 - Estimates of the parameters in IRF CO₂ (Joos et al., 2013).

τ_1 (year)	394.4
τ_2 (year)	36.54
τ_3 (year)	4.3
a_0	0.217
a_1	0.224
a_2	0.282
a_3	0.276

Table SI III.7 - Estimates of the parameters in IRF for methane and nitrous oxide

Compound	Formula	Lifetime
Methane	CH ₄	12.4
Nitrous oxide	N ₂ O	121

Table SI III.8 - Simplified values of specific radiative forcing, A_i , in $\text{W m}^{-2} \text{ppbv}^{-1}$ from IPCC (2013) and $\text{W m}^{-2} \text{kg}^{-1}$, for carbon dioxide, methane and nitrous oxide.

Gas	Specific radiative forcing	
	$(\text{W m}^{-2} \text{kg}^{-1})$	$(\text{W m}^{-2} \text{ppbv}^{-1})$
CO ₂	1.75×10^{-15}	1.37×10^{-3}
CH ₄	1.27×10^{-13}	3.63×10^{-4}
N ₂ O	3.83×10^{-13}	3.00×10^{-3}

SI III.8 Dynamic parameters

Table SI III.9 -BD process data for dynamic assessment.

Process	Process model					
	α	β_{CO_2}	β_{N_2O}	β_{CH_4}	T	r
1 - Biomass Culture	$\alpha=0.1$	$\beta_{CO_2}=0.00$ 98647	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0109469
2 - Biomass Flocculation	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
3 - Biomass Dewatering	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
4 - Biomass Drying	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
5.1 - Oil extraction, Oil	$\alpha=0.1$	$\beta_{CO_2}=0.01$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
6 - Biodiesel Transesterification	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
7 - Biodiesel Purification	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
8 - Biodiesel Use (FU)	$\alpha=0.1$	$\beta_{CO_2}=0.00$ 7407	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=1 0	r=0.0027367
9 - Electricity Production	$\alpha=0.1$	$\beta_{CO_2}=0.00$ 857279	$\beta_{N_2O}=0.00000$ 0191596	$\beta_{CH_4}=0.0000$ 00565928	T=1 0	r=0.0027367
10 - Heat Production	$\alpha=0.1$	$\beta_{CO_2}=0.00$ 672691	$\beta_{N_2O}=0.00000$ 00241395	$\beta_{CH_4}=0.0000$ 0000679293	T=1 0	r=0.0027367
11 - CO ₂ liquid Production	$\alpha=1$	$\beta_{CO_2}=0.53$ 3227	$\beta_{N_2O}=0.00001$ 0158	$\beta_{CH_4}=0.0000$ 118854	T=1	r=0.0191571
12 - N fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.75$ 9918	$\beta_{N_2O}=0.01892$ 26	$\beta_{CH_4}=0.0000$ 211292	T=1	r=0.0191571
13 - P fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.48$ 7189	$\beta_{N_2O}=0.00007$ 4361	$\beta_{CH_4}=0.0001$ 0154	T=1	r=0.0191571
14 - Soda Production	$\alpha=1$	$\beta_{CO_2}=1.03$ 6537	$\beta_{N_2O}=0.00003$ 21786	$\beta_{CH_4}=0.0000$ 504713	T=1	r=0.0191571
15 - Methanol Production	$\alpha=1$	$\beta_{CO_2}=0.63$ 6546	$\beta_{N_2O}=0.00000$ 481761	$\beta_{CH_4}=0.0000$ 0391515	T=1	r=0.0191571
16 - Infrastructure culture	$\alpha=1$	$\beta_{CO_2}=5089$ 013.314	$\beta_{N_2O}=32.2923$ 738	$\beta_{CH_4}=17.788$ 0404	T=1 0	r=9
17 - Infrastructure dewatering	$\alpha=1$	$\beta_{CO_2}=4958$.703045	$\beta_{N_2O}=0.06059$ 976	$\beta_{CH_4}=0.0527$ 3004	T=1 0	r=9
18 - Infrastructure Drying	$\alpha=1$	$\beta_{CO_2}=3569$ 6.30461	$\beta_{N_2O}=0.43624$ 058	$\beta_{CH_4}=0.3795$ 8870	T=1 0	r=9
19 - Infrastructure Extraction	$\alpha=1$	$\beta_{CO_2}=825.$ 1790451	$\beta_{N_2O}=0.01008$ 442	$\beta_{CH_4}=0.008$ 77482	T=1 0	r=9
20 - Infrastructure Transesterification	$\alpha=1$	$\beta_{CO_2}=3311$.905049	$\beta_{N_2O}=0.04047$ 442	$\beta_{CH_4}=0.0352$ 1826	T=1 0	r=9
21 - Infrastructure Purification	$\alpha=1$	$\beta_{CO_2}=1062$.942499	$\beta_{N_2O}=0.01299$ 010	$\beta_{CH_4}=0.0113$ 0316	T=1 0	r=9
22 - Transport lorry	$\alpha=1$	$\beta_{CO_2}=0.18$ 59580	$\beta_{N_2O}=0.00000$ 27263	$\beta_{CH_4}=0.0000$ 00711112	T=1	r=0.0027367
23 - Transport freight	$\alpha=1$	$\beta_{CO_2}=0.03$ 7548702	$\beta_{N_2O}=0.00000$ 101579	$\beta_{CH_4}=0.0000$ 0110939	T=1	r=0.0054734
24 - Transport barge	$\alpha=1$	$\beta_{CO_2}=0.04$ 4427345	$\beta_{N_2O}=0.00000$ 337913	$\beta_{CH_4}=0.0000$ 00231824	T=1	r=0.0191571

Table SI III.10 -BD supply chain data for dynamic assessment

Producer	Consumer	Supply model	
7 - Biodiesel Purification	8 - Biodiesel Use	a = -0.026455	$\delta = 0.2472633$
22 - Transport lorry	8 - Biodiesel Use	a = -0.05291	$\delta = 0$
6 - Biodiesel Transesterification	7 - Biodiesel Purification	a = -1	$\delta = 0.0109469$
10 - Heat Production	7 - Biodiesel Purification	cont (a = -4.45471)	$\delta = 0$
21 - Infrastructure Purification	7 - Biodiesel Purification	a = -1.7241E-8	$\delta = 1$
5.1 - Oil extraction, Oil	6 - Biodiesel Transesterification	a = -1.0475	$\delta = 0.0109469$
15 - Methanol Production	6 - Biodiesel Transesterification	a = -0.11598	$\delta = 0.2308429$
9 - Electricity Production	6 - Biodiesel Transesterification	cont (a = -0.0185)	$\delta = 0$
10 - Heat Production	6 - Biodiesel Transesterification	cont (a = -1.34021)	$\delta = 0$
20 - Infrastructure Transesterification	6 - Biodiesel Transesterification	a = -1.7241E-8	$\delta = 1$
4 – Biomass Drying	5.1 - Oil extraction, Oil	a = -1	$\delta = 0.0109469$
11 - CO2 liquid Production	5.1 - Oil extraction, Oil	a = -0.1	$\delta = 0.2308429$
9 - Electricity Production	5.1 - Oil extraction, Oil	cont (a = -1.31383)	$\delta = 0$
10 - Heat Production	5.1 - Oil extraction, Oil	cont (a = -11.69995)	$\delta = 0$
19 - Infrastructure Extraction	5.1 - Oil extraction, Oil	a = -4.20884E-9	$\delta = 1$
3 – Biomass Dewatering	4 – Biomass Drying	a = -1	$\delta = 0.0109469$
9 - Electricity Production	4 – Biomass Drying	cont (a = -1.33199)	$\delta = 0$
18 - Infrastructure Drying	4 – Biomass Drying	a = (-4.21E-9)	$\delta = 1$
2 – Biomass Flocculation	3 – Biomass Dewatering	a = -1	$\delta = 0.0109469$
9 - Electricity Production	3 – Biomass Dewatering	cont (a = -0.00691)	$\delta = 0$
17 - Infrastructure dewatering	3 - Biomass Dewatering	a = -4.2088E-9	$\delta = 1$
1 - Biomass Culture	2 – Biomass Flocculation	a = -1.111111	$\delta = 0.0027367$
14 - Soda Production	2 – Biomass Flocculation	a = -0.0008	$\delta = 0.2308429$
9 - Electricity Production	2 – Biomass Flocculation	cont (a = -0.41025)	$\delta = 0$
9 - Electricity Production	1 - Biomass Culture	cont (a = -0.227)	$\delta = 0$
12 - N fertiliser Production	1 - Biomass Culture	a = -0.03282	$\delta = 0.2308429$
13 - P fertiliser Production	1 - Biomass Culture	a = -0.01047	$\delta = 0.2308429$
16 - Infrastructure culture	1 - Biomass Culture	a = -3.788E-9	$\delta = 1$
22 - Transport lorry	1 - Biomass Culture	a = -0.004329	$\delta = 0$
23 - Transport freight	1 - Biomass Culture	a = -0.004329	$\delta = 0$
24 - Transport barge	1 - Biomass Culture	a = -0.033726	$\delta = 0$
22 - Transport lorry	5.1 - Oil extraction, Oil	a = -0.002	$\delta = 0$
22 - Transport lorry	2 – Biomass Flocculation	a = -0.0000016	$\delta = 0$
22 - Transport lorry	6 - Biodiesel Transesterification	a = -0.034794	$\delta = 0$
24 - Transport barge	6 - Biodiesel Transesterification	a = -0.52191	$\delta = 0$

Table SI III.11- Heat BD cogeneration process data for dynamic assessment

Process	Process model					
	α	β_{CO_2}	β_{N_2O}	β_{CH_4}	T	r
1 - Biomass Culture	$\alpha=0.1$	$\beta_{CO_2}=0.0098647$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0109469
2 - Biomass Flocculation	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027367
3 - Biomass Dewatering	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027367
4 - Biomass Drying	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027367
5.2 - Oil extraction, Biomass	$\alpha=0.1$	$\beta_{CO_2}=0.01$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027367
9 - Electricity Production	$\alpha=0.1$	$\beta_{CO_2}=0.00857279$	$\beta_{N_2O}=0.000000$ 191596	$\beta_{CH_4}=0.000000$ 0565928	T=10	r=0.0027367
10 - Heat Production	$\alpha=0.1$	$\beta_{CO_2}=0.00672691$	$\beta_{N_2O}=0.000000$ 0241395	$\beta_{CH_4}=0.000000$ 000679293	T=10	r=0.0027367
11 - CO ₂ liquid Production	$\alpha=1$	$\beta_{CO_2}=0.533227$	$\beta_{N_2O}=0.000010$ 158	$\beta_{CH_4}=0.00001$ 18854	T=1	r=0.0191571
12 - N fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.759918$	$\beta_{N_2O}=0.018922$ 6	$\beta_{CH_4}=0.00002$ 11292	T=1	r=0.0191571
13 - P fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.487189$	$\beta_{N_2O}=0.000074$ 361	$\beta_{CH_4}=0.00010$ 154	T=1	r=0.0191571
14 - Soda Production	$\alpha=1$	$\beta_{CO_2}=1.036537$	$\beta_{N_2O}=0.000032$ 1786	$\beta_{CH_4}=0.00005$ 04713	T=1	r=0.0191571
16 - Infrastructure culture	$\alpha=1$	$\beta_{CO_2}=5089013.31$ 4	$\beta_{N_2O}=32.29237$ 38	$\beta_{CH_4}=17.7880$ 404	T=10	r=9
17 - Infrastructure dewatering	$\alpha=1$	$\beta_{CO_2}=4958.70304$ 5	$\beta_{N_2O}=0.060599$ 76	$\beta_{CH_4}=0.05273$ 004	T=10	r=9
18 - Infrastructure Drying	$\alpha=1$	$\beta_{CO_2}=35696.3046$ 1	$\beta_{N_2O}=0.436240$ 58	$\beta_{CH_4}=0.37958$ 870	T=10	r=9
19 - Infrastructure Extraction	$\alpha=1$	$\beta_{CO_2}=825.179045$ 1	$\beta_{N_2O}=0.010084$ 42	$\beta_{CH_4}=0.00877$ 482	T=10	r=9
22 - Transport lorry	$\alpha=1$	$\beta_{CO_2}=0.1859580$	$\beta_{N_2O}=0.000002$ 7263	$\beta_{CH_4}=0.000000$ 0711112	T=1	r=0.0027367
23 - Transport freight	$\alpha=1$	$\beta_{CO_2}=0.03754870$ 2	$\beta_{N_2O}=0.000001$ 01579	$\beta_{CH_4}=0.000000$ 110939	T=1	r=0.0054734
24 - Transport barge	$\alpha=1$	$\beta_{CO_2}=0.04442734$ 5	$\beta_{N_2O}=0.000003$ 37913	$\beta_{CH_4}=0.000000$ 0231824	T=1	r=0.0191571
16 - Infrastructure Digester	$\alpha=1$	$\beta_{CO_2}=34598.15051$	$\beta_{N_2O}=0.134129$	$\beta_{CH_4}=0.11715$ 7	T=10	r=9
17- Infrastructure Cogeneration	$\alpha=1$	$\beta_{CO_2}=94379.78463$	$\beta_{N_2O}=1.624703$	$\beta_{CH_4}=1.33135$	T=10	r=9
18- Infrastructure Spreading	$\alpha=1$	$\beta_{CO_2}=30026.7490$ 7	$\beta_{N_2O}=0.910463$	$\beta_{CH_4}=0.17584$ 1	T=10	r=9
19 - Digestion, Methane	$\alpha=0.1$	$\beta_{CO_2}=0.255636$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027367
20 - Spreading	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0.000001$ 77517	$\beta_{CH_4}=0$	T=10	r=0.0027367
30.2 - Cogeneration, Heat	$\alpha=0.1$	$\beta_{CO_2}=0.000013209$	$\beta_{N_2O}=1.4676E-$ 7	$\beta_{CH_4}=0.000000$ 13502	T=10	r=0

Table SI III.12 -Heat BD cogeneration supply chain data for dynamic assessment

Producer	Consumer	Supply model	
4 - Biomass Drying	5.2- Oil extraction, Biomass	a = -1	$\delta = 0.0109469$
11 - CO2 liquid Production	5.2- Oil extraction, Biomass	a = -0.1	$\delta = 0.2308429$
9 - Electricity Production	5.2- Oil extraction, Biomass	cont (a = -1.313834)	$\delta = 0$
10 - Heat Production	5.2- Oil extraction, Biomass	cont (a = -11.69995)	$\delta = 0$
19 - Infrastructure Extraction	5.2- Oil extraction, Biomass	a = -4.20884E-9	$\delta = 1$
3 - Biomass Dewatering	4 - Biomass Drying	a = -1	$\delta = 0.0109469$
9 - Electricity Production	4 - Biomass Drying	cont (a = -1.33199)	$\delta = 0$
18 - Infrastructure Drying	4 - Biomass Drying	a = (-4.21E-9)	$\delta = 1$
2 - Biomass Flocculation	3 - Biomass Dewatering	a = -1	$\delta = 0.0109469$
9 - Electricity Production	3 - Biomass Dewatering	cont (a = -0.00691)	$\delta = 0$
17 - Infrastructure dewatering	3 - Biomass Dewatering	a = -4.2088E-9	$\delta = 1$
1 - Biomass Culture	2 - Biomass Flocculation	a = -1.111111	$\delta = 0.0027367$
14 - Soda Production	2 - Biomass Flocculation	a = -0.0008	$\delta = 0.2308429$
9 - Electricity Production	2 - Biomass Flocculation	cont (a = -0.41025)	$\delta = 0$
9 - Electricity Production	1 - Biomass Culture	cont (a = -0.227)	$\delta = 0$
12 - N fertiliser Production	1 - Biomass Culture	a = -0.03282	$\delta = 0.2308429$
13 - P fertiliser Production	1 - Biomass Culture	a = -0.01047	$\delta = 0.2308429$
16 - Infrastructure culture	1 - Biomass Culture	a = -3.788E-9	$\delta = 1$
22 - Transport lorry	1 - Biomass Culture	a = -0.004329	$\delta = 0$
23 - Transport freight	1 - Biomass Culture	a = -0.004329	$\delta = 0$
24 - Transport barge	1 - Biomass Culture	a = -0.033726	$\delta = 0$
22 - Transport lorry	5.2 - Oil extraction, Biomass	cont (a = -0.002)	$\delta = 0.2472633$
22 - Transport lorry	2 - Biomass Flocculation	cont (a = -0.0000016)	$\delta = 0.2472633$
25 - Infrastructure Digester	28 - Digestion, Methane	a = -0.000000300673	$\delta = 1$
26- Infrastructure Cogeneration	30.2 - Cogeneration, Heat	a = -3.18035E-10	$\delta = 1$
27- Infrastructure Spreading	29 - Spreading	a = -0.0000000038327	$\delta = 1$
5.2 - Oil extraction, Biomass	28 - Digestion, Methane	a = -5.3136	$\delta = 0.0109469$
29 - Spreading	28 - Digestion, Methane	a = -78.3981	$\delta = 0.2472633$
9 - Electricity Production	29 - Digestion, Methane	cont (a = -0.7336)	$\delta = 0$
10 - Heat Production	30 - Digestion, Methane	cont (a = -13.48163)	$\delta = 0$
28 - Digestion, Methane	30.2 - Cogeneration, Heat	cont (a = -0.020703125)	$\delta = 0$

Table SI III.13 -Electricity BD cogeneration process data for dynamic assessment

Process (infra corrected)	Process model					
	$\alpha=0$.1	β_{CO_2}	β_{N_2O}	β_{CH_4}	T	r
1 - Biomass Culture	$\beta_{CO_2}=0.00986$ 47	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.01094 69	
2 - Biomass Flocculation	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
3 - Biomass Dewatering	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
4 - Biomass Drying	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
5.2 - Oil extraction, Biomass	$\beta_{CO_2}=0.01$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
9 - Electricity Production	$\beta_{CO_2}=0.00857$ 279	$\beta_{N_2O}=0.00000019$ 1596	$\beta_{CH_4}=0.000000$ 565928	T=10	r=0.00273 67	
10 - Heat Production	$\beta_{CO_2}=0.00672$ 691	$\beta_{N_2O}=0.00000002$ 41395	$\beta_{CH_4}=0.000000$ 00679293	T=10	r=0.00273 67	
11 - CO ₂ liquid Production	$\beta_{CO_2}=0.53322$ 7	$\beta_{N_2O}=0.00001015$ 8	$\beta_{CH_4}=0.000011$ 8854	T=1	r=0.01915 71	
12 - N fertiliser Production	$\beta_{CO_2}=2.75991$ 8	$\beta_{N_2O}=0.0189226$	$\beta_{CH_4}=0.000021$ 1292	T=1	r=0.01915 71	
13 - P fertiliser Production	$\beta_{CO_2}=2.48718$ 9	$\beta_{N_2O}=0.00007436$ 1	$\beta_{CH_4}=0.000101$ 54	T=1	r=0.01915 71	
14 - Soda Production	$\beta_{CO_2}=1.03653$ 7	$\beta_{N_2O}=0.00003217$ 86	$\beta_{CH_4}=0.000050$ 4713	T=1	r=0.01915 71	
16 - Infrastructure culture	$\beta_{CO_2}=5089013$.314	$\beta_{N_2O}=32.2923738$	$\beta_{CH_4}=17.78804$ 04	T=10	r=9	
17 - Infrastructure dewatering	$\beta_{CO_2}=4958.70$ 3045	$\beta_{N_2O}=0.06059976$	$\beta_{CH_4}=0.052730$ 04	T=10	r=9	
18 - Infrastructure Drying	$\beta_{CO_2}=35696.3$ 0461	$\beta_{N_2O}=0.43624058$	$\beta_{CH_4}=0.379588$ 70	T=10	r=9	
19 - Infrastructure Extraction	$\beta_{CO_2}=825.179$ 0451	$\beta_{N_2O}=0.01008442$	$\beta_{CH_4}=0.008774$ 82	T=10	r=9	
22 - Transport lorry	$\beta_{CO_2}=0.18595$ 80	$\beta_{N_2O}=0.00000272$ 63	$\beta_{CH_4}=0.000000$ 711112	T=1	r=0.00273 67	
23 - Transport freight	$\beta_{CO_2}=0.03754$ 8702	$\beta_{N_2O}=0.00000101$ 579	$\beta_{CH_4}=0.000001$ 10939	T=1	r=0.00547 34	
24 - Transport barge	$\beta_{CO_2}=0.04442$ 7345	$\beta_{N_2O}=0.00000337$ 913	$\beta_{CH_4}=0.000000$ 231824	T=1	r=0.01915 71	
16 - Infrastructure Digester	$\beta_{CO_2}=34598.15051$	$\beta_{N_2O}=0.134129$	$\beta_{CH_4}=0.117157$	T=10	r=9	
17- Infrastructure Cogeneration	$\beta_{CO_2}=94379.78463$	$\beta_{N_2O}=1.624703$	$\beta_{CH_4}=1.33135$	T=10	r=9	
18- Infrastructure Spreading	$\beta_{CO_2}=30026.7$ 4907	$\beta_{N_2O}=0.910463$	$\beta_{CH_4}=0.175841$	T=10	r=9	
19 - Digestion, Methane	$\beta_{CO_2}=0.25563$ 6	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
20 - Spreading	$\beta_{CO_2}=0$	$\beta_{N_2O}=0.00000177$ 517	$\beta_{CH_4}=0$	T=10	r=0.00273 67	
30.1 - Cogeneration, Electricity	$\beta_{CO_2}=0.0000475508$	$\beta_{N_2O}=5.28343E-7$	$\beta_{CH_4}=0.000004$ 86075	T=10	r=0	

Table SI III.14 -Electricity BD cogeneration supply chain data for dynamic assessment

Producer	Consumer	Supply model	
4 - Biomass Drying	5.2- Oil extraction, Biomass	a = -1	$\delta = 0.0109469$
11 - CO2 liquid Production	5.2- Oil extraction, Biomass	a = -0.1	$\delta = 0.2308429$
9 - Electricity Production	5.2- Oil extraction, Biomass	cont (a = -1.313834)	$\delta = 0$
10 - Heat Production	5.2- Oil extraction, Biomass	cont (a = -11.69995)	$\delta = 0$
19 - Infrastructure Extraction	5.2- Oil extraction, Biomass	a = -4.20884E-9	$\delta = 1$
3 - Biomass Dewatering	4 - Biomass Drying	a = -1	$\delta = 0.0109469$
9 - Electricity Production	4 - Biomass Drying	cont (a = -1.33199)	$\delta = 0$
18 - Infrastructure Drying	4 - Biomass Drying	a = (-4.21E-9)	$\delta = 1$
2 - Biomass Flocculation	3 - Biomass Dewatering	a = -1	$\delta = 0.0109469$
9 - Electricity Production	3 - Biomass Dewatering	cont (a = -0.00691)	$\delta = 0$
17 - Infrastructure dewatering	3 - Biomass Dewatering	a = -4.2088E-9	$\delta = 1$
1 - Biomass Culture	2 - Biomass Flocculation	a = -1.111111	$\delta = 0.0027367$
14 - Soda Production	2 - Biomass Flocculation	a = -0.0008	$\delta = 0.2308429$
9 - Electricity Production	2 - Biomass Flocculation	cont (a = -0.41025)	$\delta = 0$
9 - Electricity Production	1 - Biomass Culture	cont (a = -0.227)	$\delta = 0$
12 - N fertiliser Production	1 - Biomass Culture	a = -0.03282	$\delta = 0.2308429$
13 - P fertiliser Production	1 - Biomass Culture	a = -0.01047	$\delta = 0.2308429$
16 - Infrastructure culture	1 - Biomass Culture	a = -3.788E-9	$\delta = 1$
22 - Transport lorry	1 - Biomass Culture	a = -0.004329	$\delta = 0$
23 - Transport freight	1 - Biomass Culture	a = -0.004329	$\delta = 0$
24 - Transport barge	1 - Biomass Culture	a = -0.033726	$\delta = 0$
22 - Transport lorry	5.2 - Oil extraction, Biomass	cont (a = -0.002)	$\delta = 0.2472633$
22 - Transport lorry	2 - Biomass Flocculation	cont (a = -0.0000016)	$\delta = 0.2472633$
25 - Infrastructure Digester	28 - Digestion, Methane	a = -0.0000000300673	$\delta = 1$
26- Infrastructure Cogeneration	30.1 - Cogeneration, Electricity	a = -1.14492E-9	$\delta = 1$
27- Infrastructure Spreading	29 - Spreading	a = -0.00000000038327	$\delta = 1$
5.2 - Oil extraction, Biomass	28 - Digestion, Methane	a = -5.3136	$\delta = 0.0109469$
29 - Spreading	28 - Digestion, Methane	a = -78.3981	$\delta = 0.2472633$
9 - Electricity Production	29 - Digestion, Methane	cont (a = -0.7336)	$\delta = 0$
10 - Heat Production	30 - Digestion, Methane	cont (a = -13.48163)	$\delta = 0$
28 - Digestion, Methane	30.1 - Cogeneration, Electricity	cont (a = -0.020703125)	$\delta = 0$

Table SI III.15 -Electricity BG cogeneration process data for dynamic assessment

Process (infra corrected)	Process model					
	α	β_{CO_2}	β_{N_2O}	β_{CH_4}	T	r
1 - Biomass Culture	$\alpha=0.1$	$\beta_{CO_2}=0.009$ 8647	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T= 10	r=0.0109 469
2 – Biomass Flocculation	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T= 10	r=0.0027 367
3 – Biomass Dewatering	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T= 10	r=0.0027 367
9 - Electricity Production	$\alpha=0.1$	$\beta_{CO_2}=0.008$ 57279	$\beta_{N_2O}=0.00000019$ 1596	$\beta_{CH_4}=0.00000056$ 5928	T= 10	r=0.0027 367
10 - Heat Production	$\alpha=0.1$	$\beta_{CO_2}=0.006$ 72691	$\beta_{N_2O}=0.00000002$ 41395	$\beta_{CH_4}=0.00000000$ 679293	T= 10	r=0.0027 367
12 - N fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.759$ 918	$\beta_{N_2O}=0.0189226$	$\beta_{CH_4}=0.00002112$ 92	T= 1	r=0.0191 571
13 - P fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.487$ 189	$\beta_{N_2O}=0.00007436$ 1	$\beta_{CH_4}=0.00010154$	T= 1	r=0.0191 571
14 - Soda Production	$\alpha=1$	$\beta_{CO_2}=1.036$ 537	$\beta_{N_2O}=0.00003217$ 86	$\beta_{CH_4}=0.00005047$ 13	T= 1	r=0.0191 571
16 - Infrastructure culture	$\alpha=1$	$\beta_{CO_2}=50890$ 13.314	$\beta_{N_2O}=32.2923738$	$\beta_{CH_4}=17.7880404$	T= 10	r=9
17 - Infrastructure dewatering	$\alpha=1$	$\beta_{CO_2}=4958.$ 703045	$\beta_{N_2O}=0.06059976$	$\beta_{CH_4}=0.05273004$	T= 10	r=9
22 - Transport lorry	$\alpha=1$	$\beta_{CO_2}=0.185$ 9580	$\beta_{N_2O}=0.00000272$ 63	$\beta_{CH_4}=0.00000071$ 1112	T= 1	r=0.0027 367
23 - Transport freight	$\alpha=1$	$\beta_{CO_2}=0.037$ 548702	$\beta_{N_2O}=0.00000101$ 579	$\beta_{CH_4}=0.00000110$ 939	T= 1	r=0.0054 734
24 - Transport barge	$\alpha=1$	$\beta_{CO_2}=0.044$ 427345	$\beta_{N_2O}=0.00000337$ 913	$\beta_{CH_4}=0.00000023$ 1824	T= 1	r=0.0191 571
16 - Infrastructure Digester	$\alpha=1$	$\beta_{CO_2}=34598.1505$ 1	$\beta_{N_2O}=0.134129$	$\beta_{CH_4}=0.117157$	T= 10	r=9
17- Infrastructure Cogeneration	$\alpha=1$	$\beta_{CO_2}=94379.7846$ 3	$\beta_{N_2O}=1.624703$	$\beta_{CH_4}=1.33135$	T= 10	r=9
18- Infrastructure Spreading	$\alpha=1$	$\beta_{CO_2}=30026$.74907	$\beta_{N_2O}=0.910463$	$\beta_{CH_4}=0.175841$	T= 10	r=9
19 - Digestion, Methane	$\alpha=0.1$	$\beta_{CO_2}=0.255$ 636	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T= 10	r=0.0027 367
20 - Spreading	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0.00000177$ 517	$\beta_{CH_4}=0$	T= 10	r=0.0027 367
30.2 - Cogeneration, Electricity	$\alpha=0.1$	$\beta_{CO_2}=0.00001320$ 9	$\beta_{N_2O}=1.4676E-7$	$\beta_{CH_4}=0.00000135$ 02	T= 10	r=0

Table SI III.16 -Electricity BG cogeneration supply chain data for dynamic assessment

Producer	Consumer	Supply model	
2 – Biomass Flocculation	3 – Biomass Dewatering	a = -1	$\delta = 0.0109469$
9 - Electricity Production	3 – Biomass Dewatering	cont (a = -0.00691)	$\delta = 0$
17 - Infrastructure dewatering	3 – Biomass Dewatering	a = -4.2088E-9	$\delta = 1$
1 - Biomass Culture	2 – Biomass Flocculation	a = -1.111111	$\delta = 0.0027367$
14 - Soda Production	2 – Biomass Flocculation	a = -0.0008	$\delta = 0.2308429$
9 - Electricity Production	2 – Biomass Flocculation	cont (a = -0.41025)	$\delta = 0$
9 - Electricity Production	1 - Biomass Culture	cont (a = -0.227)	$\delta = 0$
12 - N fertiliser Production	1 - Biomass Culture	a = -0.03282	$\delta = 0.2308429$
13 - P fertiliser Production	1 - Biomass Culture	a = -0.01047	$\delta = 0.2308429$
16 - Infrastructure culture	1 - Biomass Culture	a = -3.788E-9	$\delta = 1$
22 - Transport lorry	1 - Biomass Culture	a = -0.004329	$\delta = 0$
23 - Transport freight	1 - Biomass Culture	a = -0.004329	$\delta = 0$
24 - Transport barge	1 - Biomass Culture	a = -0.033726	$\delta = 0$
22 - Transport lorry	2 – Biomass Flocculation	cont (a = -0.0000016)	$\delta = 0.2472633$
25 - Infrastructure Digester	28 - Digestion, Methane	a = -0.0000000300673	$\delta = 1$
26- Infrastructure Cogeneration	30.2 - Cogeneration, Heat	a = -3.18035E-10	$\delta = 1$
27- Infrastructure Spreading	29 - Spreading	a = -0.00000000038327	$\delta = 1$
3 – Biomass Dewatering	28 - Digestion, Methane	a = -1.68786	$\delta = 0.0109469$
29 - Spreading	28 - Digestion, Methane	a = -23.8538	$\delta = 0.2472633$
9 - Electricity Production	29 - Digestion, Methane	cont (a = -0.7336)	$\delta = 0$
10 - Heat Production	30 - Digestion, Methane	cont (a = -13.48163)	$\delta = 0$
28 - Digestion, Methane	30.2 - Cogeneration, Electricity	cont (a = -0.020703125)	$\delta = 0$

Table SI III.17 -Heat BG cogeneration process data for dynamic assessment

Process	Process model					
1 - Biomass Culture	$\alpha=0.1$	$\beta_{CO_2}=0.009$ 8647	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0109 469
2 – Biomass Flocculation	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027 367
3 – Biomass Dewatering	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027 367
9 - Electricity Production	$\alpha=0.1$	$\beta_{CO_2}=0.008$ 57279	$\beta_{N_2O}=0.00000019$ 1596	$\beta_{CH_4}=0.00000005$ 65928	T=10	r=0.0027 367
10 - Heat Production	$\alpha=0.1$	$\beta_{CO_2}=0.006$ 72691	$\beta_{N_2O}=0.00000002$ 41395	$\beta_{CH_4}=0.00000000$ 0679293	T=10	r=0.0027 367
12 - N fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.759$ 918	$\beta_{N_2O}=0.0189226$	$\beta_{CH_4}=0.0000211$ 292	T=1	r=0.0191 571
13 - P fertiliser Production	$\alpha=1$	$\beta_{CO_2}=2.487$ 189	$\beta_{N_2O}=0.00007436$ 1	$\beta_{CH_4}=0.0001015$ 4	T=1	r=0.0191 571
14 - Soda Production	$\alpha=1$	$\beta_{CO_2}=1.036$ 537	$\beta_{N_2O}=0.00003217$ 86	$\beta_{CH_4}=0.0000504$ 713	T=1	r=0.0191 571
16 - Infrastructure culture	$\alpha=1$	$\beta_{CO_2}=50890$ 13.314	$\beta_{N_2O}=32.2923738$	$\beta_{CH_4}=17.788040$ 4	T=10	r=9
17 - Infrastructure dewatering	$\alpha=1$	$\beta_{CO_2}=4958.$ 703045	$\beta_{N_2O}=0.06059976$	$\beta_{CH_4}=0.0527300$ 4	T=10	r=9
22 - Transport lorry	$\alpha=1$	$\beta_{CO_2}=0.185$ 9580	$\beta_{N_2O}=0.00000272$ 63	$\beta_{CH_4}=0.0000007$ 11112	T=1	r=0.0027 367
23 - Transport freight	$\alpha=1$	$\beta_{CO_2}=0.037$ 548702	$\beta_{N_2O}=0.00000101$ 579	$\beta_{CH_4}=0.0000011$ 0939	T=1	r=0.0054 734
24 - Transport barge	$\alpha=1$	$\beta_{CO_2}=0.044$ 427345	$\beta_{N_2O}=0.00000337$ 913	$\beta_{CH_4}=0.0000002$ 31824	T=1	r=0.0191 571
16 - Infrastructure Digester	$\alpha=1$	$\beta_{CO_2}=34598.1505$ 1	$\beta_{N_2O}=0.134129$	$\beta_{CH_4}=0.117157$	T=10	r=9
17- Infrastructure Cogeneration	$\alpha=1$	$\beta_{CO_2}=94379.7846$ 3	$\beta_{N_2O}=1.624703$	$\beta_{CH_4}=1.33135$	T=10	r=9
18- Infrastructure Spreading	$\alpha=1$	$\beta_{CO_2}=30026$.74907	$\beta_{N_2O}=0.910463$	$\beta_{CH_4}=0.175841$	T=10	r=9
19 - Digestion, Methane	$\alpha=0.1$	$\beta_{CO_2}=0.255$ 636	$\beta_{N_2O}=0$	$\beta_{CH_4}=0$	T=10	r=0.0027 367
20 - Spreading	$\alpha=0.1$	$\beta_{CO_2}=0$	$\beta_{N_2O}=0.00000177$ 517	$\beta_{CH_4}=0$	T=10	r=0.0027 367
30.2 - Cogeneration, Heat	$\alpha=0.1$	$\beta_{CO_2}=0.00001320$ 9	$\beta_{N_2O}=1.4676E-7$	$\beta_{CH_4}=0.0000013$ 502	T=10	r=0

Table SI III.18 -Heat BG cogeneration supply chain data for dynamic assessment

Producer	Consumer	Supply model	
2 – Biomass Flocculation	3 – Biomass Dewatering	a = -1	$\delta = 0.0109469$
9 - Electricity Production	3 – Biomass Dewatering	cont (a = -0.00691)	$\delta = 0$
17 - Infrastructure dewatering	3 – Biomass Dewatering	a = -4.2088E-9	$\delta = 1$
1 - Biomass Culture	2 – Biomass Flocculation	a = -1.111111	$\delta = 0.0027367$
14 - Soda Production	2 – Biomass Flocculation	a = -0.0008	$\delta = 0.2308429$
9 - Electricity Production	2 – Biomass Flocculation	cont (a = -0.41025)	$\delta = 0$
9 - Electricity Production	1 - Biomass Culture	cont (a = -0.227)	$\delta = 0$
12 - N fertiliser Production	1 - Biomass Culture	a = -0.03282	$\delta = 0.2308429$
13 - P fertiliser Production	1 - Biomass Culture	a = -0.01047	$\delta = 0.2308429$
16 - Infrastructure culture	1 - Biomass Culture	a = -3.788E-9	$\delta = 1$
22 - Transport lorry	1 - Biomass Culture	a = -0.004329	$\delta = 0$
23 - Transport freight	1 - Biomass Culture	a = -0.004329	$\delta = 0$
24 - Transport barge	1 - Biomass Culture	a = -0.033726	$\delta = 0$
22 - Transport lorry	2 – Biomass Flocculation	cont (a = -0.0000016)	$\delta = 0.2472633$
25 - Infrastructure Digester	28 - Digestion, Methane	a = -0.0000000300673	$\delta = 1$
26- Infrastructure Cogeneration	30.2 - Cogeneration, Heat	a = -3.18035E-10	$\delta = 1$
27- Infrastructure Spreading	29 - Spreading	a = -0.00000000038327	$\delta = 1$
3 – Biomass Dewatering	28 - Digestion, Methane	a = -1.68786	$\delta = 0.0109469$
29 - Spreading	28 - Digestion, Methane	a = -23.8538	$\delta = 0.2472633$
9 - Electricity Production	29 - Digestion, Methane	cont (a = -0.7336)	$\delta = 0$
10 - Heat Production	30 - Digestion, Methane	cont (a = -13.48163)	$\delta = 0$
28 - Digestion, Methane	30.2 - Cogeneration, Heat	cont (a = -0.020703125)	$\delta = 0$

Table SI III.19 – Absolute mid-point impacts from Recipe method

Impact	Unit	BD	Elec BD	Elec BG	Heat BD	Heat BG
ALOP	m2a	4.30E-04	1.09E-02	2.03E-03	5.17E-04	3.23E-04
GWP100	kg CO2-Eq	1.45E-01	2.60E+00	3.58E-01	1.23E-01	5.61E-02
FDP	kg oil-Eq	2.17E-02	3.98E-01	3.86E-02	1.88E-02	4.44E-03
FETPinf	kg 1,4-DCB	1.77E-04	4.05E-03	1.32E-03	1.91E-04	8.62E-05
FEP	kg P-Eq	8.83E-06	3.41E-04	1.41E-04	1.61E-05	1.11E-05
HTPinf	kg 1,4-DCB	1.14E-02	2.82E-01	7.17E-02	1.33E-02	5.61E-03
IRP_HE	kg U235-Eq	1.10E-01	3.09E+00	2.92E-01	1.46E-01	4.30E-02
METPinf	kg 1,4-DCB	2.01E-04	4.72E-03	1.32E-03	2.23E-04	9.79E-05
MEP	kg N-Eq	7.06E-05	3.00E-03	4.15E-04	1.42E-04	4.95E-05
MDP	kg Fe-Eq	2.14E-03	4.59E-02	1.59E-02	2.17E-03	1.28E-03
NLTP	m2	1.45E-05	2.38E-04	2.95E-05	1.12E-05	3.30E-06
ODPinf	kg CFC-11-	6.92E-09	1.23E-07	1.11E-08	5.82E-09	1.36E-09
PMFP	kg PM10-Eq	7.44E-05	8.48E-03	8.20E-04	4.00E-04	1.23E-04
POFP	kg NMVOC	2.12E-04	2.78E-03	5.54E-04	1.31E-04	6.67E-05
TAP100	kg SO2-Eq	1.95E-04	5.87E-02	5.06E-03	2.77E-03	7.82E-04
TETPinf	kg 1,4-DCB	5.26E-06	1.04E-04	1.29E-05	4.91E-06	1.98E-06
ULOP	m2a	2.98E-04	4.14E-03	6.18E-04	1.95E-04	9.74E-05
WDP	m3	7.75E-04	2.05E-02	1.93E-03	9.69E-04	3.10E-04

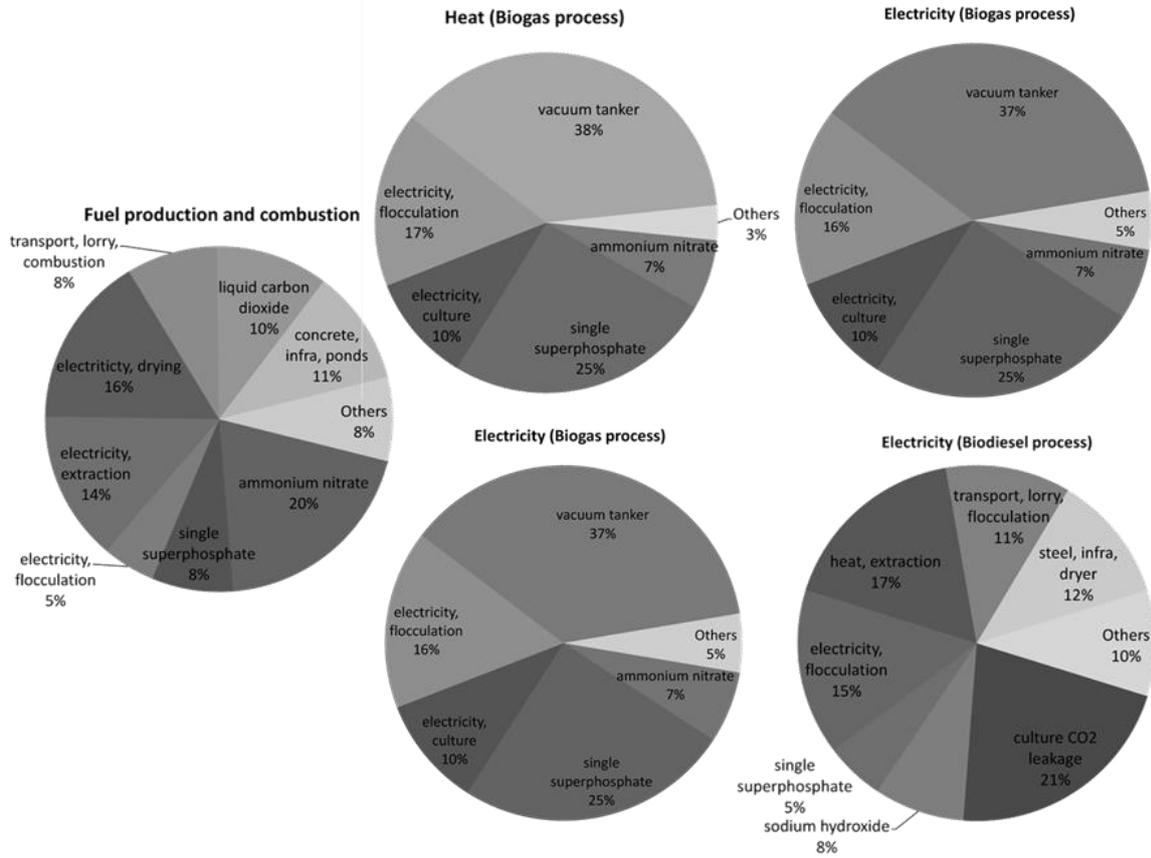


Figure SII.3 – Agricultural land occupation potential

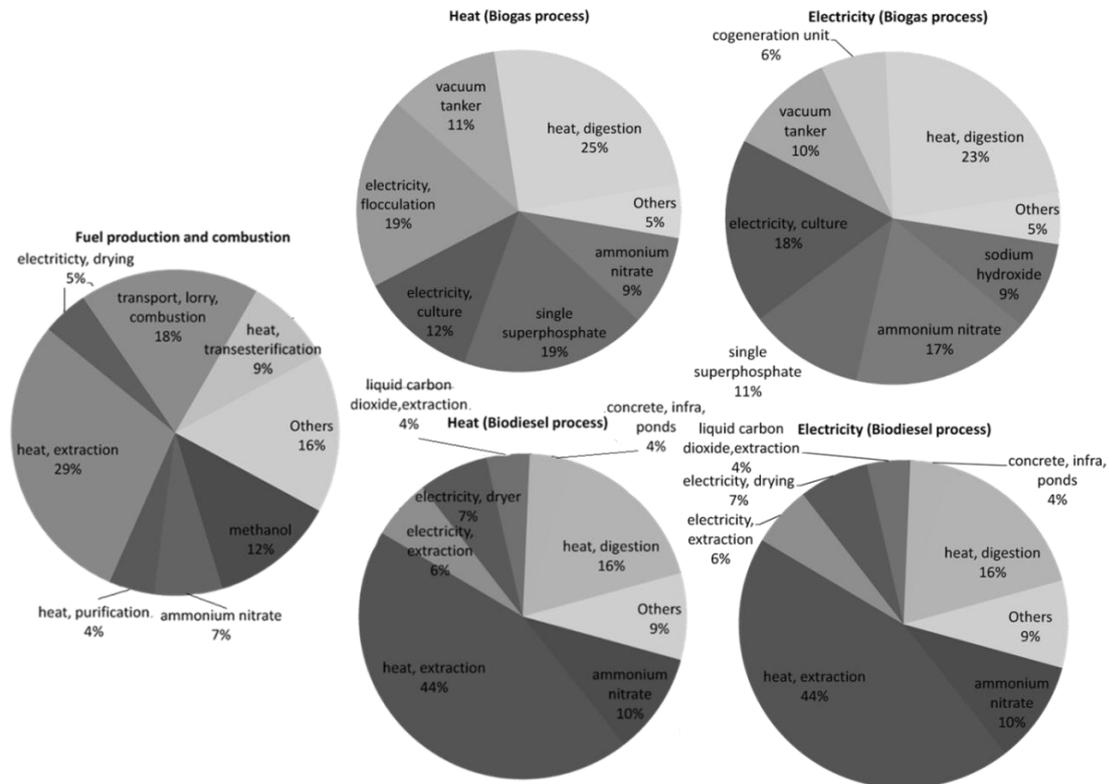


Figure SI III.4 – Fossil depletion potential

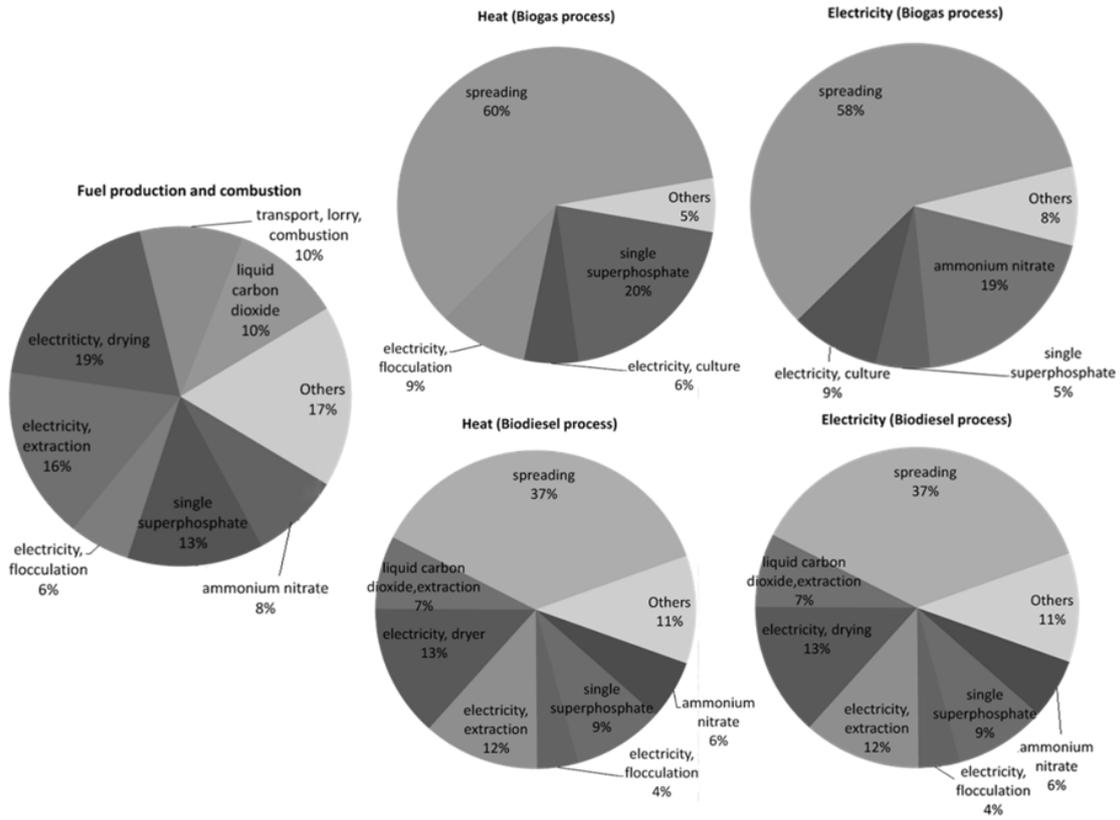


Figure SI III.5 – Freshwater eutrophication potential

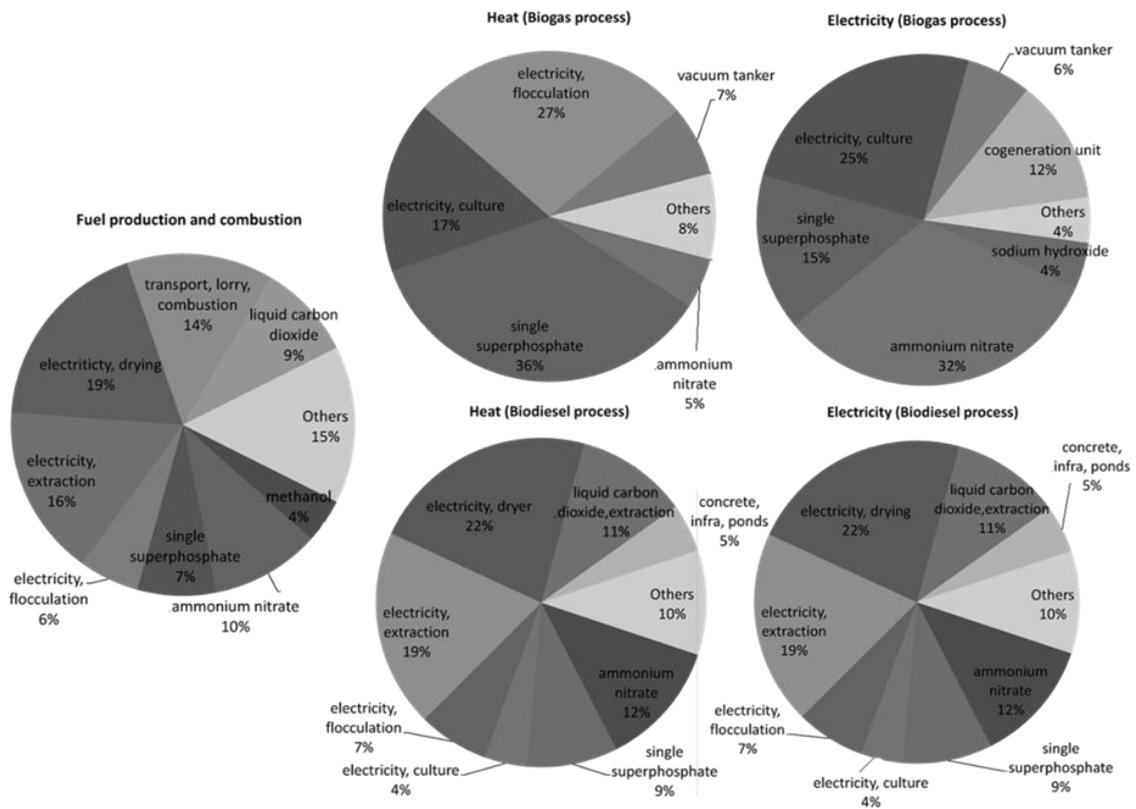


Figure SI III.6 – Freshwater ecotoxicity potential

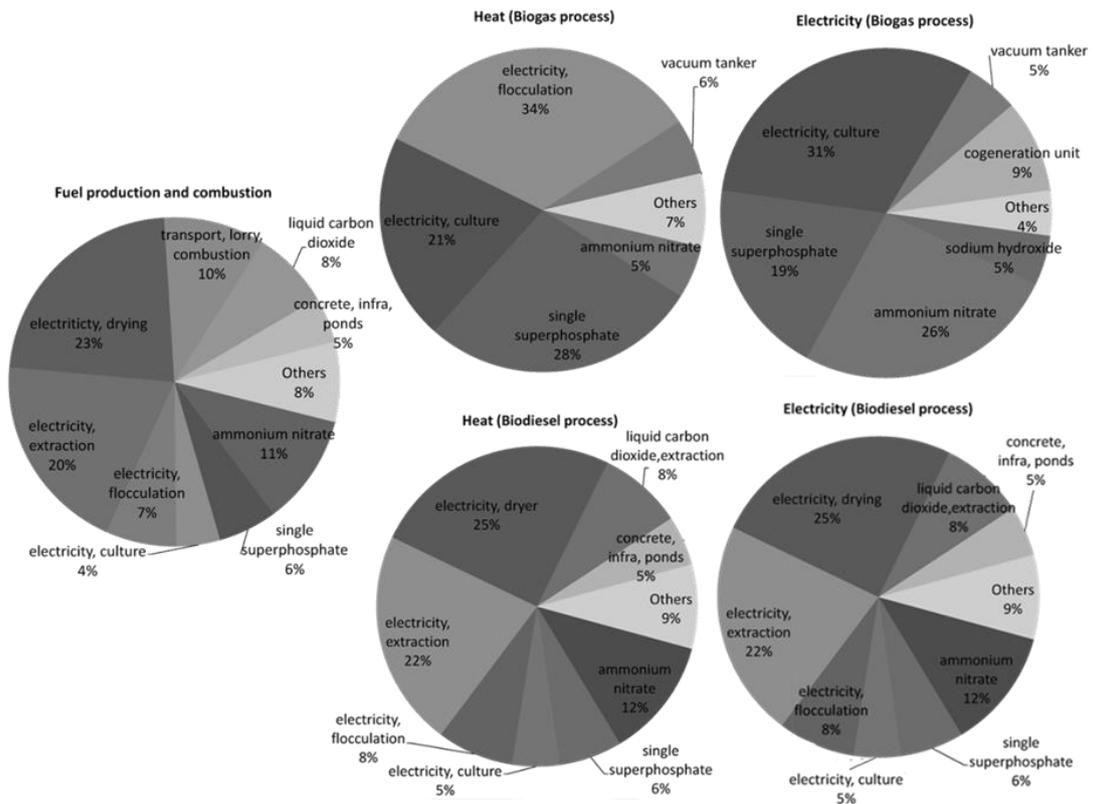


Figure SI III.7 - Human toxicity potential

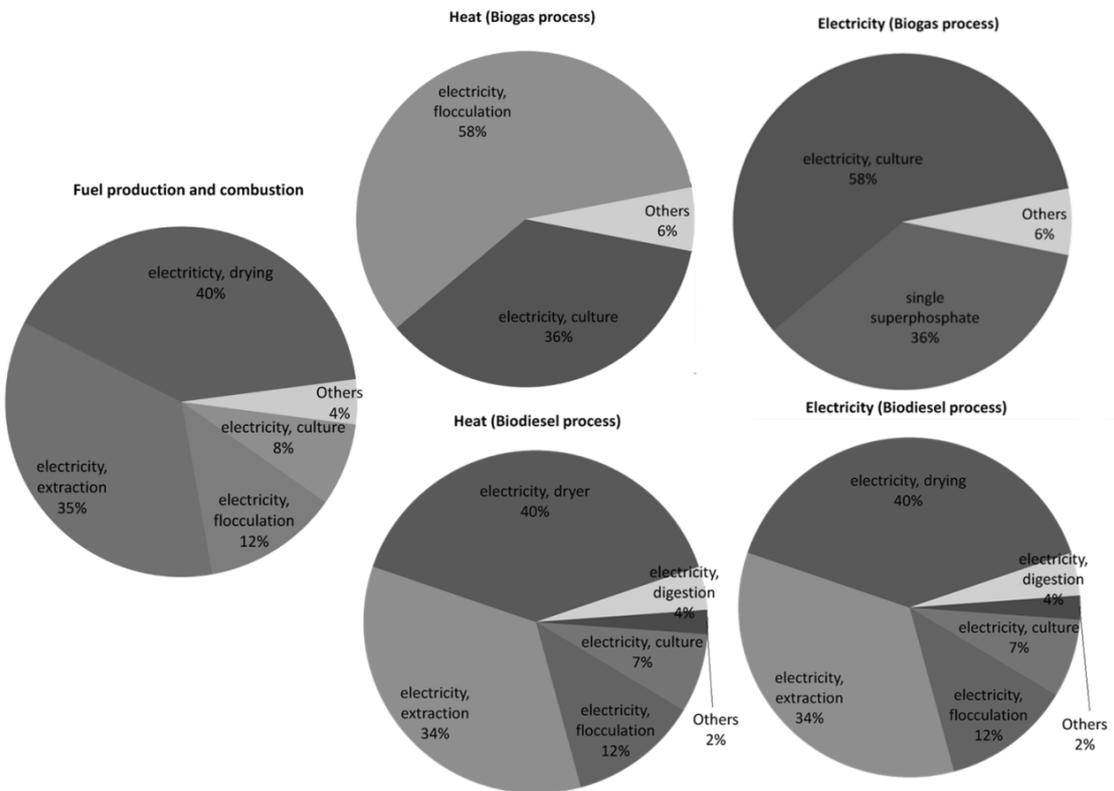


Figure SI III.8 - Ionising radiation potential

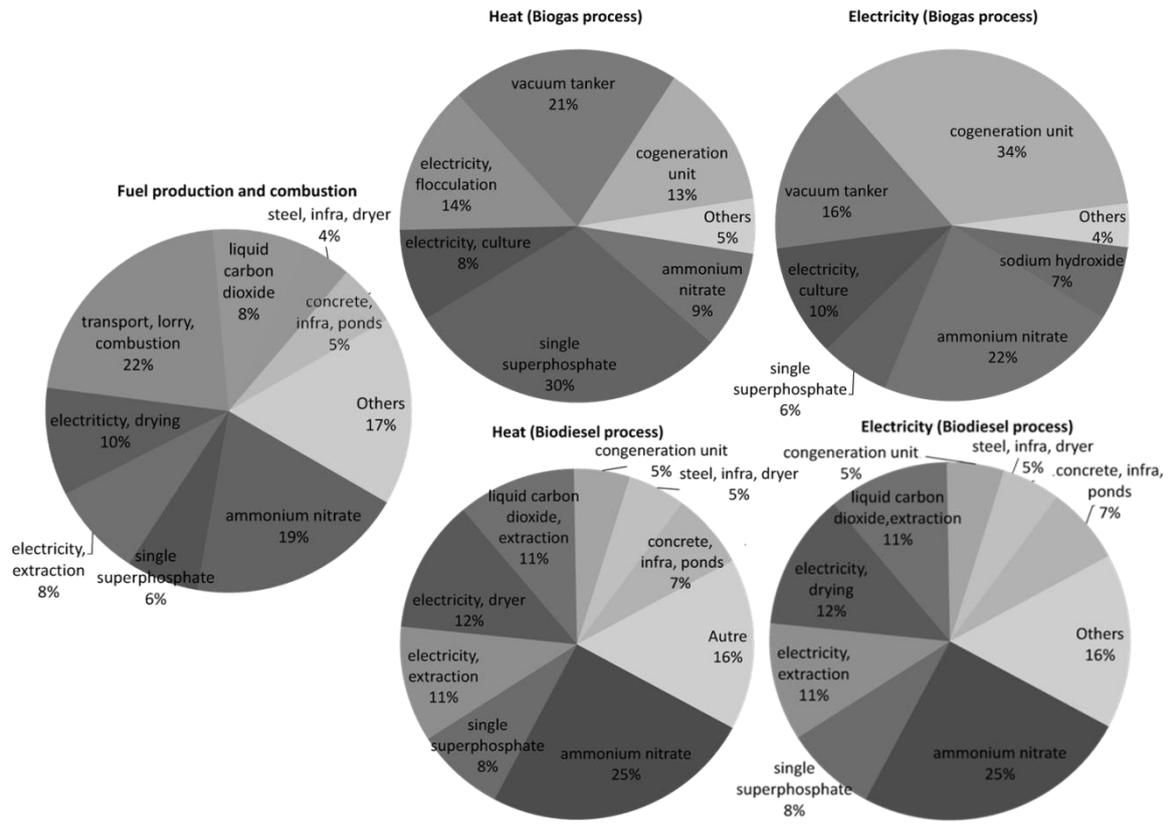


Figure SI III.9 – Metal depletion potential

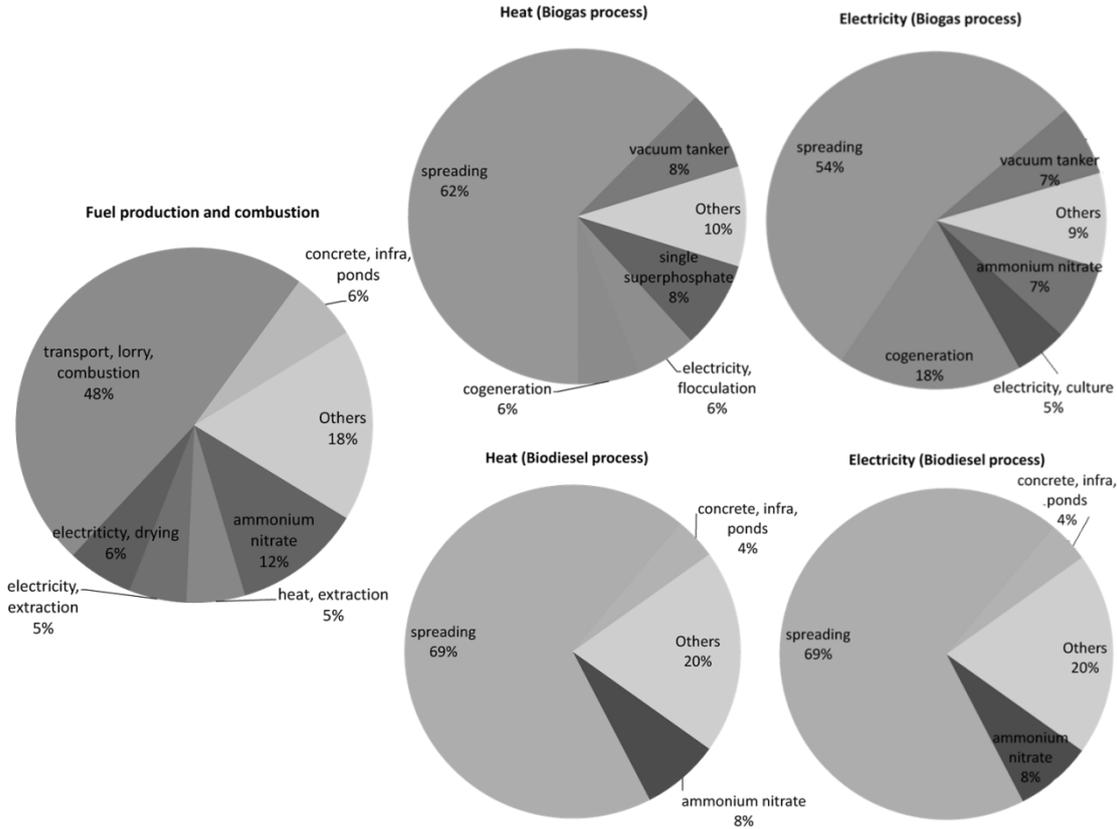


Figure SI III.10 – Marine eutrophication potential (kg N eq)

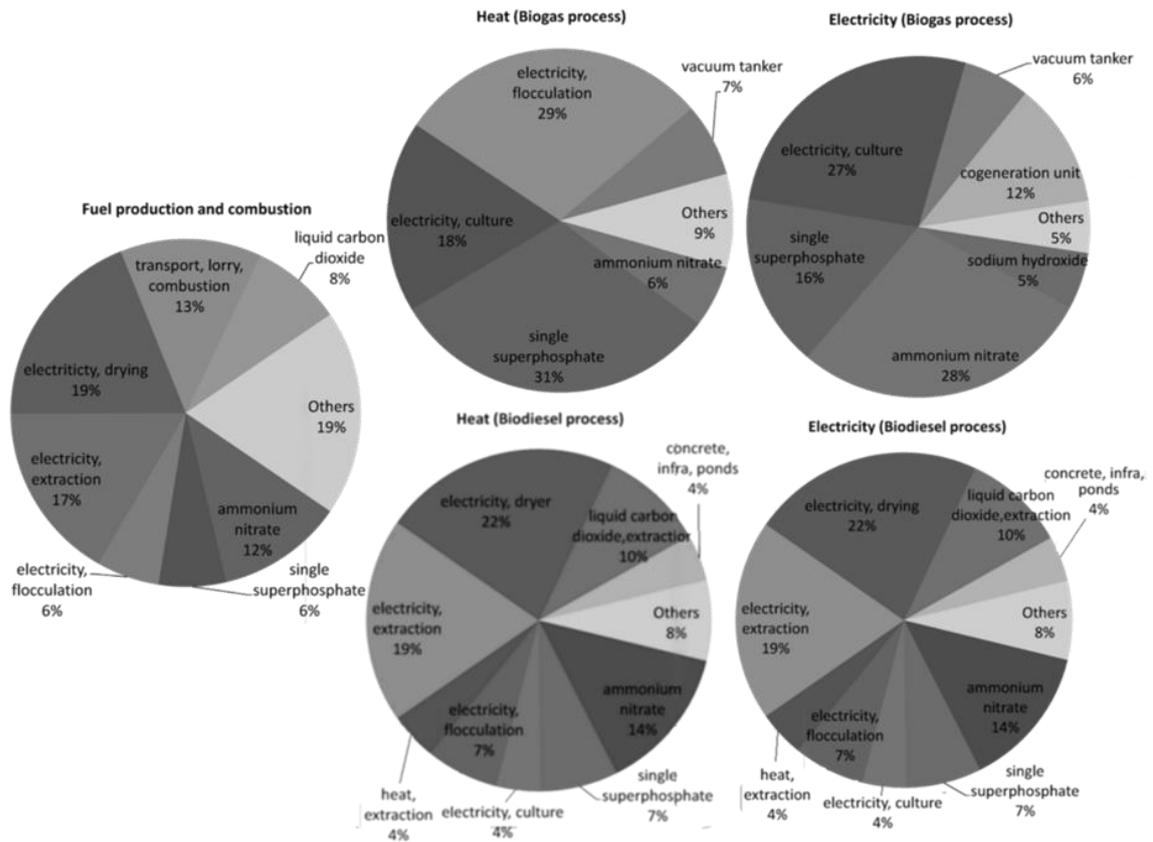


Figure SI III.11 - Marine ecotoxicity potential

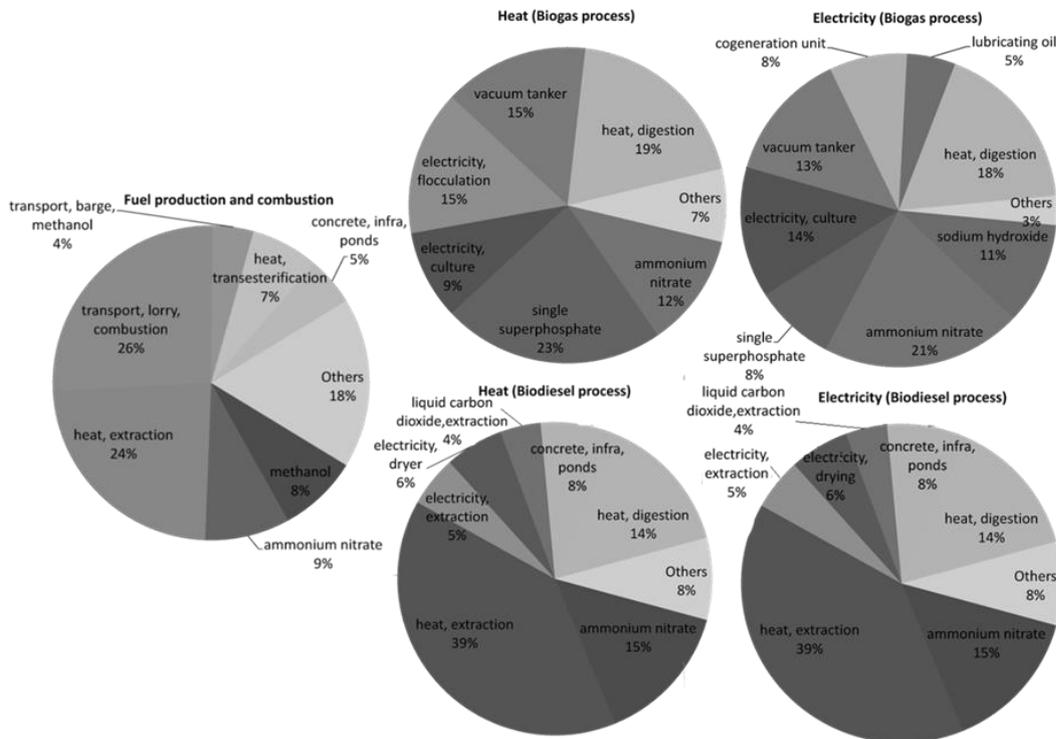


Figure SI III.12 – Natural land transformation potential

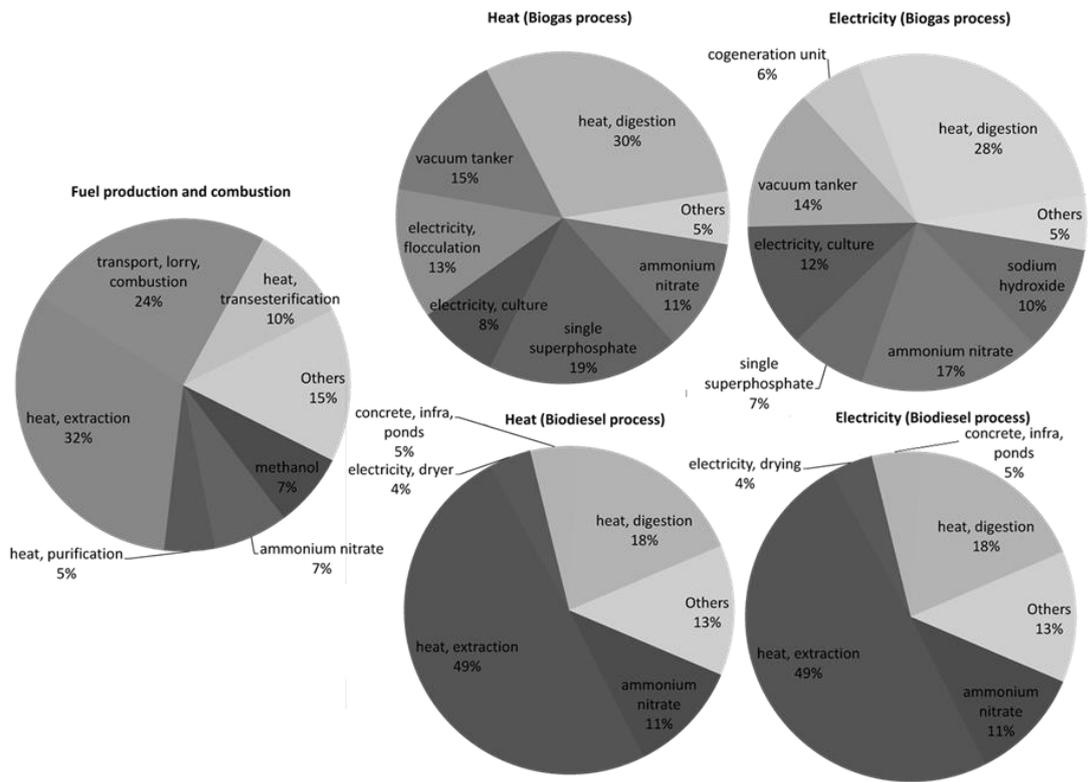


Figure SI III.13 – Ozone depletion potential

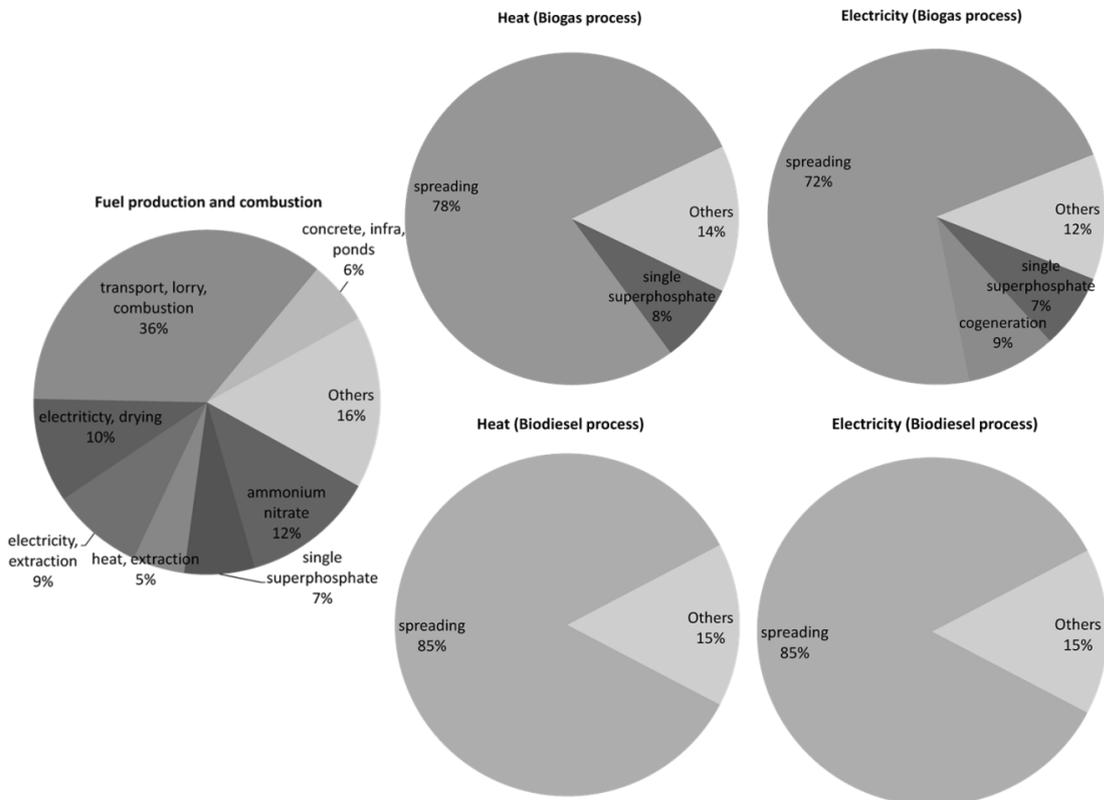


Figure SI III.14 – Particulate matter formation potential

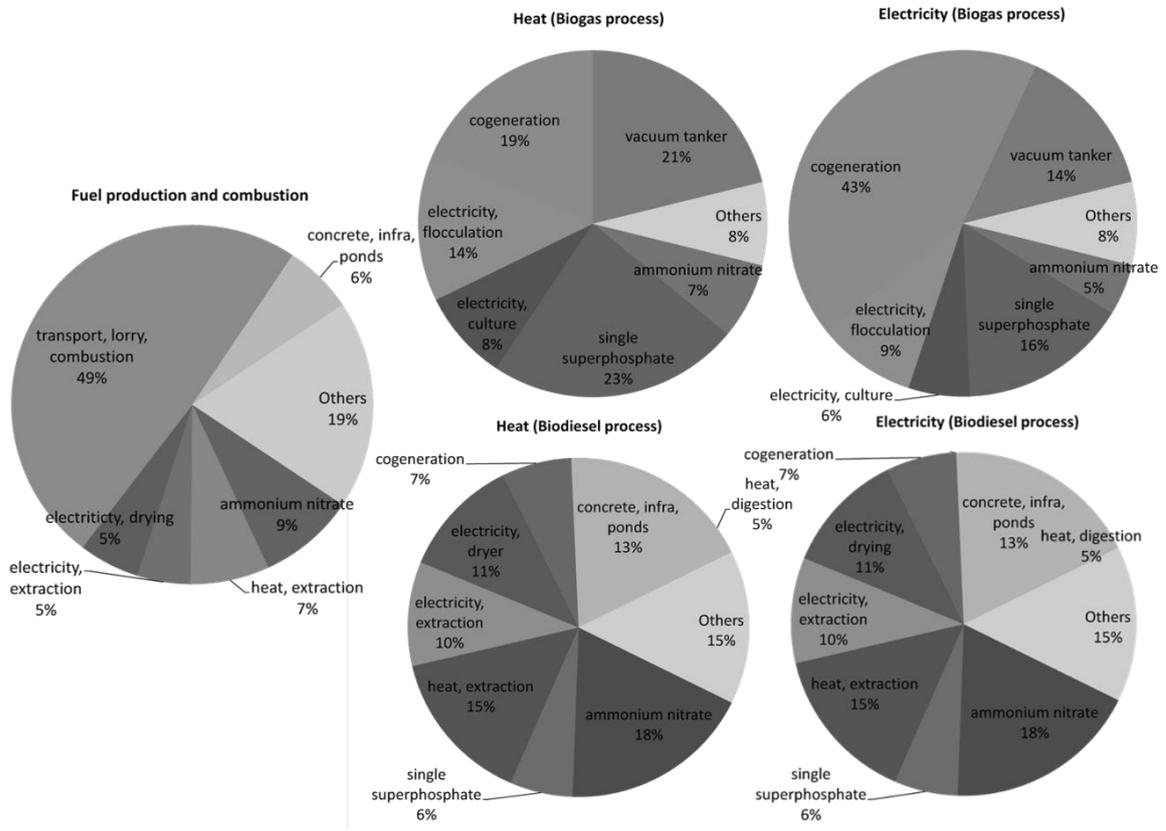


Figure SI III.15 – Photochemical oxidant formation potential

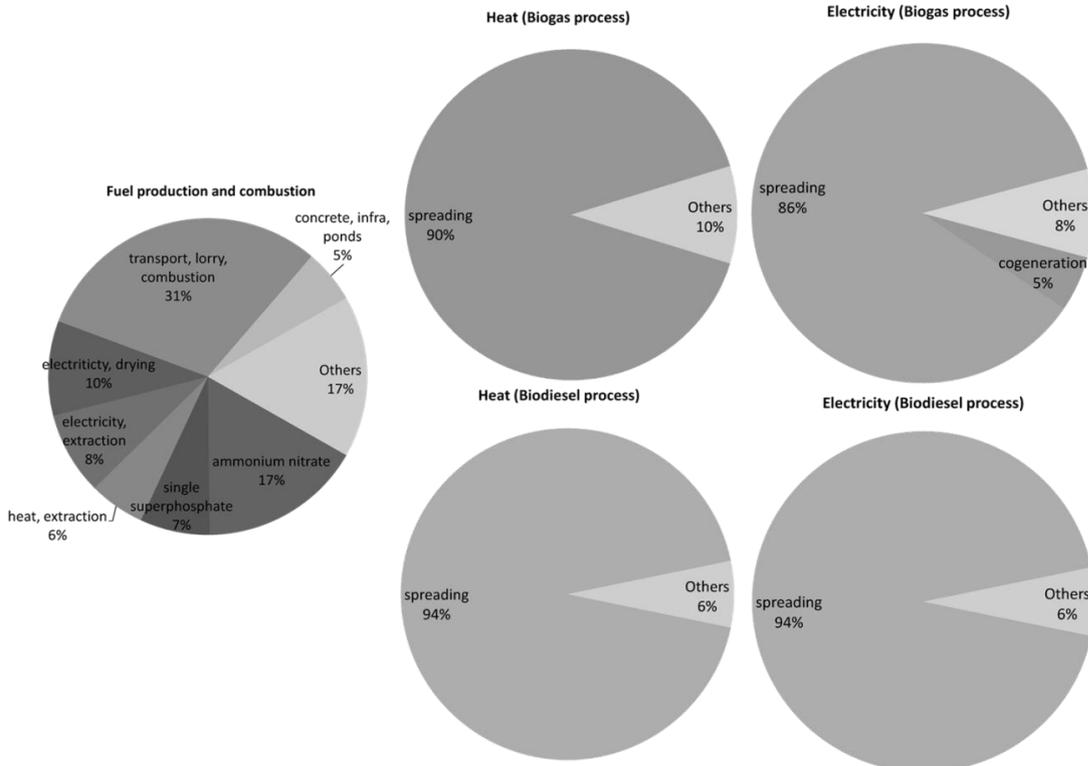


Figure SI III.16 - Terrestrial acidification potential

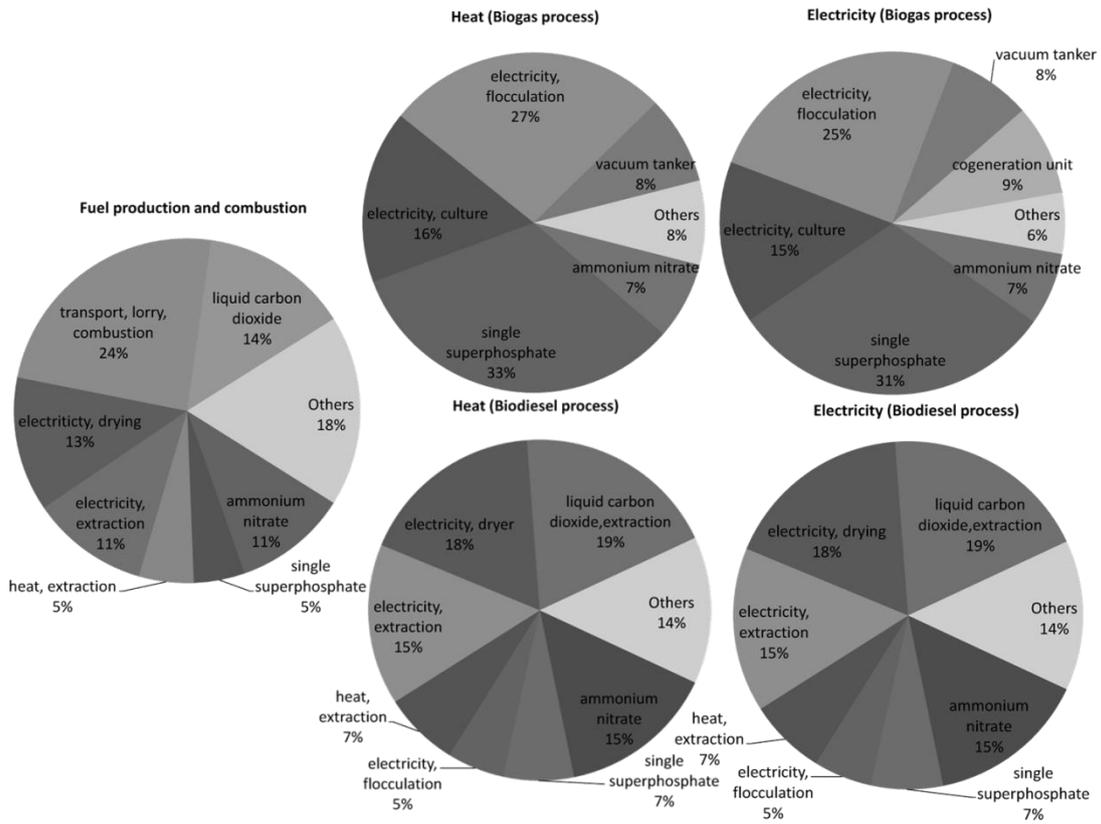


Figure SI III.17 – Terrestrial ecotoxicity potential

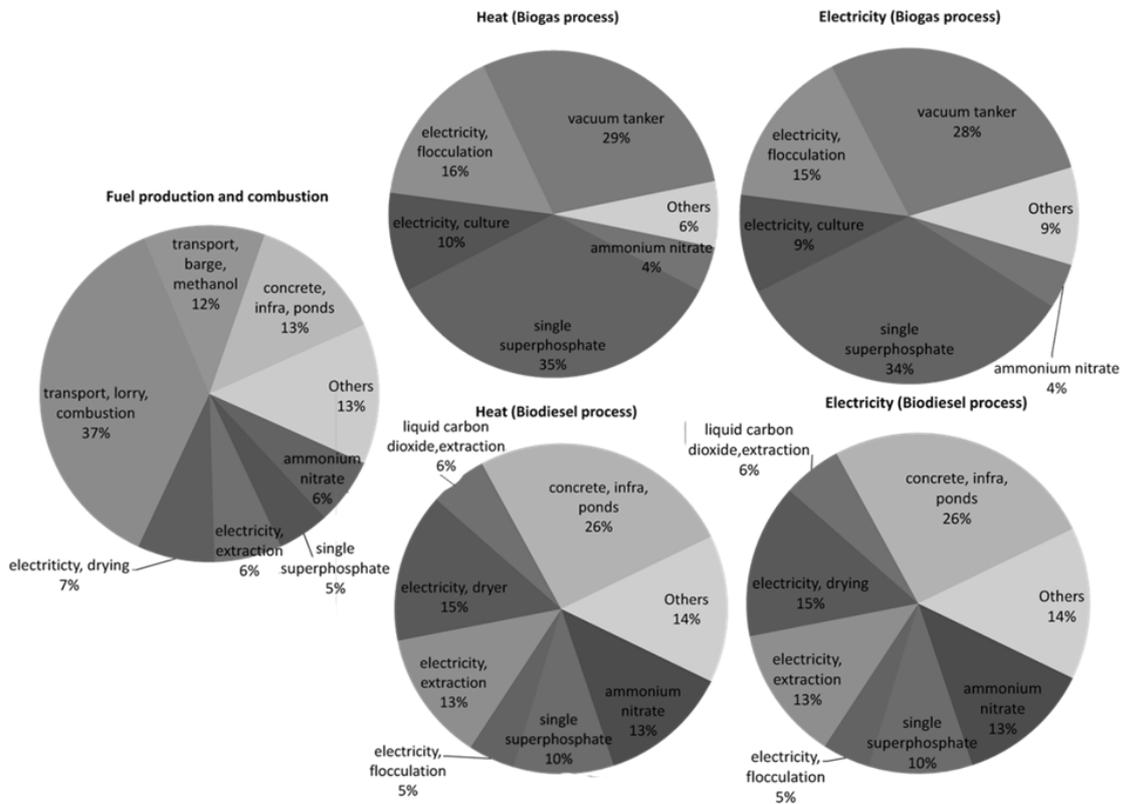


Figure SI III.18 – Urban land occupation potential

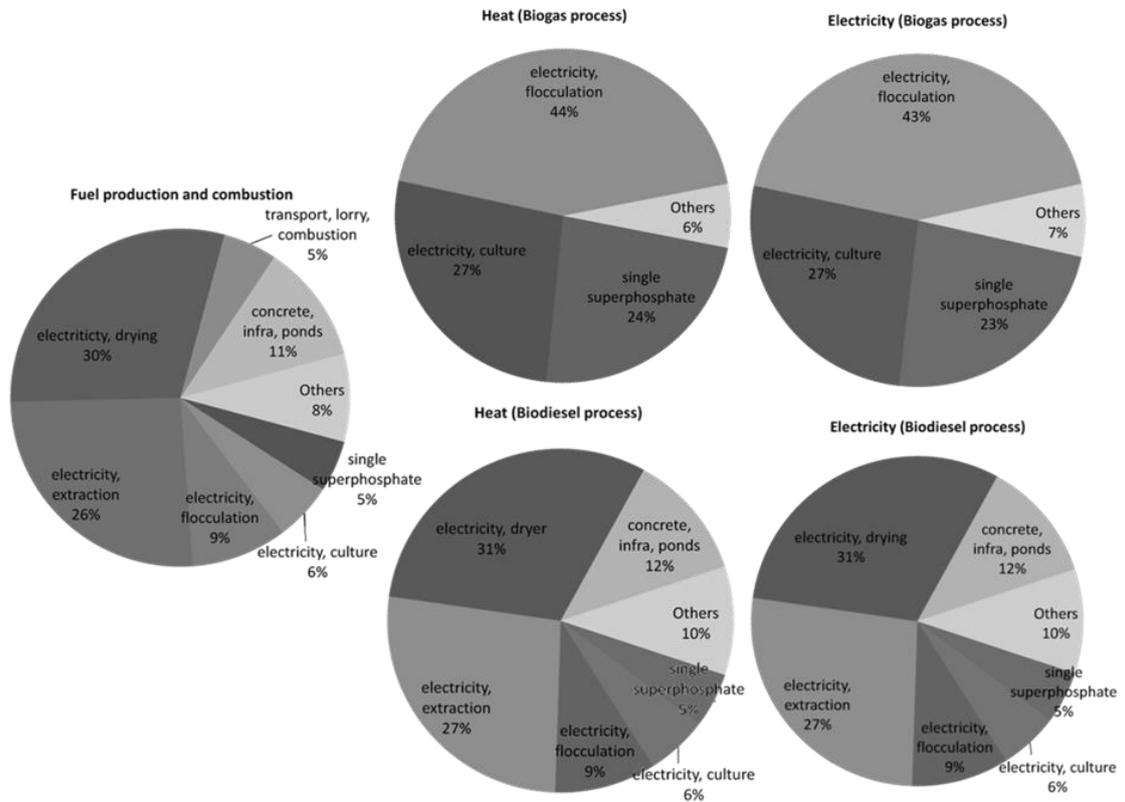


Figure SI III.19 – Water depletion potential

SI III.9 Contribution of CO₂, CH₄ and N₂O in dynamic climate change evaluation

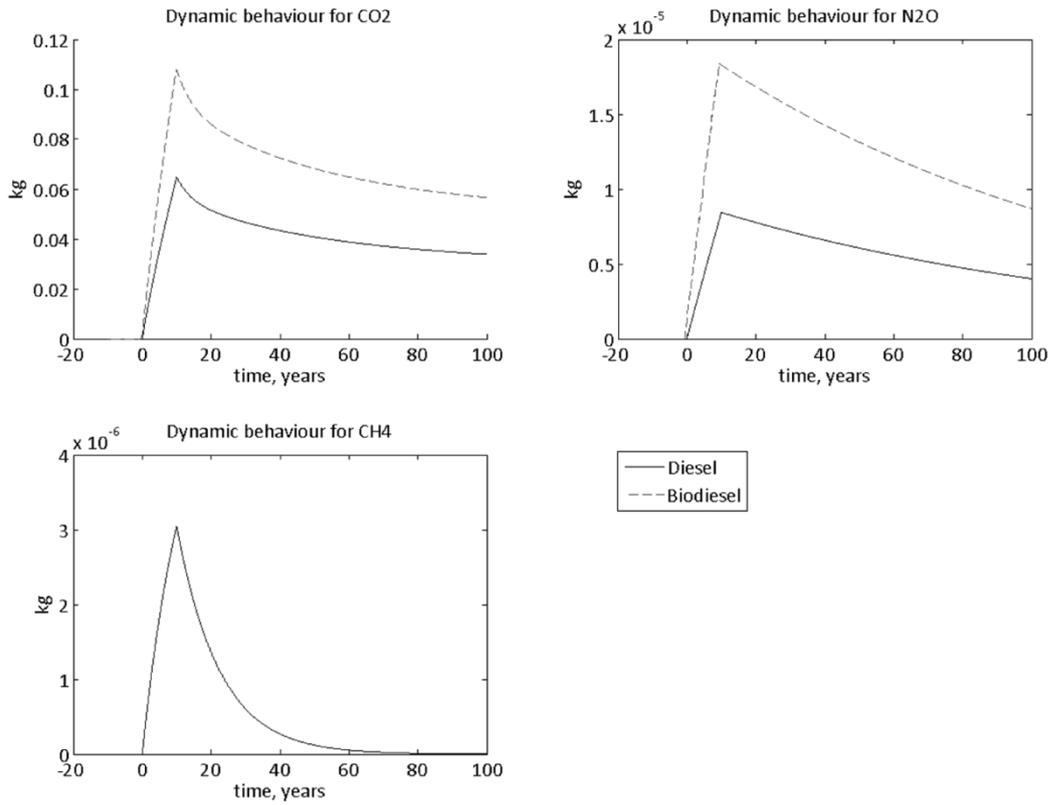


Figure SI III.20 – Dynamic behaviour of CO₂, CH₄ and N₂O for fuel production

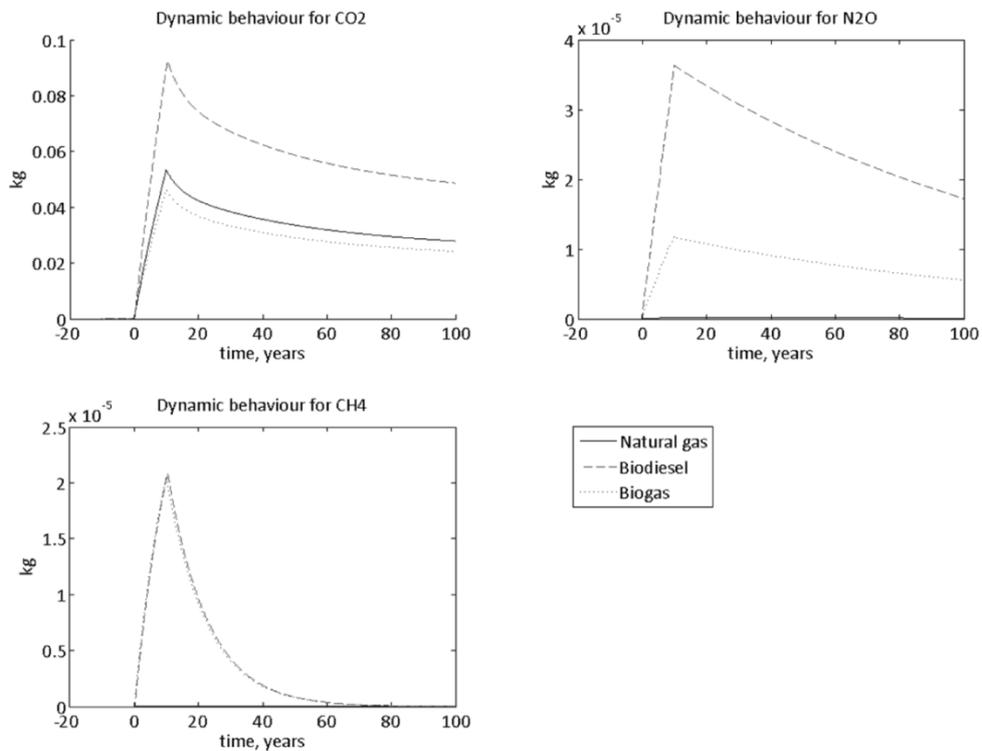


Figure SI III.21 – Dynamic behaviour of CO₂, CH₄ and N₂O for electricity production

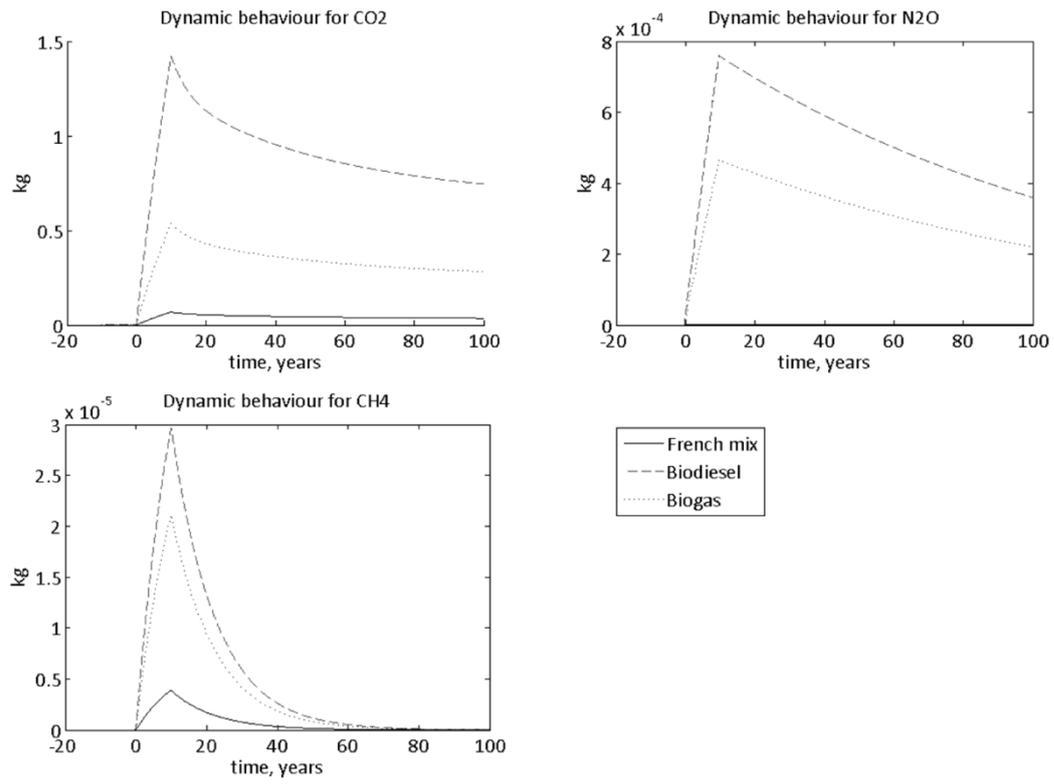


Figure SI III.22 – Dynamic behaviour of CO₂, CH₄ and N₂O for heat production

SI IV Operational integration of time dependent toxicity impact category in dynamic LCA

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SI IV.1 Compatibility of substances in ecoinvent 3.2 and USEtox® 2.0

USEtox® 2.0 contains 27 inorganic substances but none match with the substances in ecoinvent dataset. In USEtox® 2.0 metals are presented with their oxidation state while in ecoinvent they are presented in their elemental form. SimaPro LCA software proposes an adaptation in which the substances from ecoinvent 3.2 database are correlated to the ionic form presented in USEtox® 2.0. This correspondence is presented in table SI IV.1.

Table SI IV.1 – Correspondence between inorganic substances presented in SimaPro® and USEtox® 2.0, proposed by SimaPro® LCA software

Name ecoinvent, SimaPro	Name Usetox® 2.0
Silver	Ag(I)
	Al(III)
Arsenic III	As(III)
Arsenic, ion	As(V)
Arsenic	As(V)
Barium	Ba(II)
Beryllium	Be(II)
Cadmium	Cd(II)
	Co(II)
Chromium III	Cr(III)
Chromium VI	Cr(VI)
	Cs(I)
Copper	Cu(II)
	Fe(II)
	Fe(III)
Mercury	Hg(II)
	Mn(II)
Molybdenum	Mo(VI)
Nickel	Ni(II)
Lead	Pb(II)
Antimony III	Sb(III)
Antimony V	Sb(V)
Antimony	Sb(V)
Antimony, ion	Sb(V)
	Se(IV)
	Sn(II)
	Sr(II)
Thallium	Tl(I)
Vanadium	V(V)
Zinc	Zn(II)

USEtox® 2.0 presents 3077 organic substances and 2880 match with the substances in ecoinvent dataset. As the name of substances might vary from one database to another, the correspondence between them was made by means of their CAS number.

SI IV.2 Compatibility of compartments in ecoinvent 3.2 and USEtox® 2.0

Compartments in ecoinvent database and USEtox® model are addressed differently. An adaptation has to be made in order to use ecoinvent 3.2 data in USEtox® 2.0 model.

Table SI IV.2 – Correspondence between compartments in ecoinvent 3.2 and USEtox® 2.

USEtox® 2 compartments	Ecoinvent 3 compartments
Urban air	Air emission, high population density/ air emission, unspecified (50%)
Rural air	Air emission, low population density / air emission, lower stratosphere & troposphere / air emission, low population density, long-term / air emission, unspecified (50%)
Freshwater	Water emission, river / water emission, lake / water emission, unspecified / water emission, river, long-term / water emission, ground water (only in human toxicity) / water emission, ground water long term (only in human toxicity)
Sea water	Water emission, ocean
Natural soil	Soil emission, forestry / soil emission, industrial / soil emission, unspecified / water emission, ground water (only in ecotoxicity) / water emission, ground water long-term (only in ecotoxicity)
Agricultural soil	Soil emission, agriculture

SI IV.3 Grape production : ecoinvent 3.2 dataset

Table SI IV.3 – Ecoinvent 3.2 dataset for the process “grape production”

	Value	Unit
Reference Products		
Grape	1	Kg
Emissions to Environment		
Compartment: air		
Ammonia	4.86E-05	Kg
Dinitrogen monoxide	3.91E-05	Kg
Nitrogen oxides	8.22E-06	Kg
Water	0.10372	m3
Compartment: soil		
Cadmium	5.21E-08	Kg
Chromium	-3.93E-07	Kg
Copper	-1.20E-06	Kg
Lead	5.87E-07	Kg
Nickel	-3.31E-08	Kg
Pesticides, unspecified	0.0005	Kg
Zinc	-8.14E-07	Kg
Compartment: water		
Nitrate	0.0026571	Kg
Phosphate	4.96E-07	Kg
Phosphorus	1.74E-06	Kg
Water	0.058384	m3
Water	0.014596	m3
Resources from Environment		
natural resource		
Energy, gross calorific value, in biomass	3.6698	MJ
Occupation, permanent crop, irrigated, intensive	0.333	m2*year
Transformation, from permanent crop, irrigated, intensive	0.333	m2
Transformation, to permanent crop, irrigated, intensive	0.333	m2
Processes from Technosphere		
ammonium nitrate, as N	0.002	Kg
electricity, low voltage	0.09	kWh
fertilising, by broadcaster	0.000733	Ha
Irrigation	0.1767	m3
pesticide, unspecified	0.0005	Kg
phosphate fertiliser, as P2O5	0.00133	Kg
potassium sulfate, as K2O	0.00433	Kg

Between the environmental interventions, it is noticed the presence of negative emissions. Nemecek et al. (2007) shows that the calculation of these emissions are based on the balance of all inputs (fertilizers, pesticides, seed and deposition) and outputs (exported biomass, leaching and erosion) related to the “agriculture soil” multiplied by the allocation factor. The final result of this calculation can lead to a negative value of emission to “agriculture soil”.

SI IV.4 Grape production : modified dataset

The modified data set was used in this work: pesticides were added as explained in the main document, and negative values (as mentioned here above) were set to zero.

Table SI IV.4 – Modified dataset for the process “grape production”

	Value	Unit
Reference Products		
Grape	1	Kg
Emissions to Environment		
Compartment: air		
Ammonia	4.86E-05	Kg
Dinitrogen monoxide	3.91E-05	Kg
Nitrogen oxides	8.22E-06	Kg
Water	0.10372	m3
Compartment: soil		
Cadmium	5.21E-08	Kg
Lead	5.87E-07	Kg
Copper	9.1E-06	Kg
Pesticides, unspecified	0.0005	Kg
Metaldehyde	0.0000059	Kg
Mancozeb	0.0000351	Kg
Glyphosate	0.0000672	Kg
Chlorothalonil	0.0000102	Kg
Aclonifen	0.0000058	Kg
Pendimethalin	0.0000066	Kg
Metolachlor	0.0000145	Kg
Isoproturon	0.0000124	Kg
Napropamide	0.0000046	Kg
Dimethenamide	0.0000055	Kg
Metamitron	0.0000039	Kg
Folpet	0.0000116	Kg

	Value	Unit
Compartment: water		
Nitrate	0.0026571	Kg
Phosphate	4.96E-07	Kg
Phosphorus	1.74E-06	Kg
Water	0.058384	m3
Water	0.014596	m3
Resources from Environment		
natural resource		
Energy, gross calorific value, in biomass	3.6698	MJ
Occupation, permanent crop, irrigated, intensive	0.333	m2*year
Transformation, from permanent crop, irrigated, intensive	0.333	m2
Transformation, to permanent crop, irrigated, intensive	0.333	m2
Processes from Technosphere		
ammonium nitrate, as N	0.002	Kg
electricity, low voltage	0.09	kWh
fertilising, by broadcaster	0.000733	Ha
Irrigation	0.1767	m3
phosphate fertiliser, as P2O5	0.00133	Kg
potassium sulfate, as K2O	0.00433	Kg
Metaldehyde	0.0000059	Kg
Mancozeb	0.0000351	Kg
Glyphosate	0.0000672	Kg
Chlorothalonil	0.0000102	Kg
Aclonifen	0.0000058	Kg
Pendimethalin	0.0000066	Kg
Metolachlor	0.0000145	Kg
Isoproturon	0.0000124	Kg
Napropamide	0.0000046	Kg
Dimethenamide	0.0000055	Kg
Metamitron	0.0000039	Kg
Folpet	0.0000116	Kg

SI IV.5 Conventional toxicity results for the testbed case “grape production” per substances, USEtox®

Table SI IV.5 – Conventional toxicity results per substance, obtained with USEtox® 2.0

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-can (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
1-Butanol	Air	high. pop.	1.7E-12	0.0E+00	8.9E-20	2.2E-13
1-Butanol	Water	river	4.9E-09	0.0E+00	1.6E-16	2.2E-08
1-Pentanol	Air	high. pop.	1.1E-12	0.0E+00	0.0E+00	2.7E-13
1-Pentanol	Water	river	2.6E-12	0.0E+00	0.0E+00	3.2E-11
1-Propanol	Air	high. pop.	2.3E-09	0.0E+00	0.0E+00	2.2E-10
1-Propanol	Air	low. pop.	1.3E-16	0.0E+00	0.0E+00	1.2E-17
1-Propanol	Water	river	5.6E-12	0.0E+00	0.0E+00	1.3E-11
1,4-Butanediol	Air	high. pop.	4.9E-12	0.0E+00	0.0E+00	4.3E-12
1,4-Butanediol	Water	river	9.6E-12	0.0E+00	0.0E+00	7.0E-11
2-Methyl-1-propanol	Air	high. pop.	2.7E-12	0.0E+00	5.7E-20	5.6E-13
2-Methyl-1-propanol	Water	river	6.5E-12	0.0E+00	1.0E-19	4.2E-11
2-Methyl-4-chlorophenoxyacetic acid	Air	low. pop.	8.5E-14	0.0E+00	1.1E-18	6.5E-12
2-Methyl-4-chlorophenoxyacetic acid	Water	groundwater	1.3E-14	0.0E+00	3.2E-19	1.6E-12
2-Methyl-4-chlorophenoxyacetic acid	Water	river	1.9E-13	0.0E+00	4.7E-18	3.5E-10
2-Methyl-4-chlorophenoxyacetic acid	Soil	agricultural	6.1E-11	0.0E+00	1.5E-15	7.6E-09
2-Propanol	Air		1.0E-11	0.0E+00	0.0E+00	8.0E-13
2-Propanol	Air	high. pop.	9.8E-09	0.0E+00	0.0E+00	7.8E-10
2-Propanol	Air	low. pop.	2.0E-12	0.0E+00	0.0E+00	1.6E-13
2-Propanol	Water	river	1.9E-11	0.0E+00	0.0E+00	3.5E-11
2,4-D	Air	low. pop.	5.0E-11	0.0E+00	7.8E-17	1.6E-09
2,4-D	Soil	agricultural	4.5E-06	0.0E+00	4.6E-12	1.2E-04
2,4-D, dimethylamine salt	Air	low. pop.	4.1E-14	0.0E+00	0.0E+00	1.7E-11
4-Methyl-2-pentanol	Water	river	6.2E-18	0.0E+00	0.0E+00	5.4E-17
4-Methyl-2-pentanone	Air	low. pop.	4.5E-14	0.0E+00	8.8E-24	1.0E-15
4-Methyl-2-pentanone	Water		3.4E-11	0.0E+00	3.5E-20	9.9E-11
Acenaphthene	Air		9.9E-15	8.2E-21	2.9E-22	3.7E-14

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-can (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Acenaphthene	Air	high. pop.	7.8E-16	1.2E-21	4.3E-23	3.0E-15
Acenaphthene	Air	low. pop.	3.4E-12	3.6E-19	1.3E-20	1.3E-11
Acenaphthene	Water	ocean	2.1E-13	1.4E-19	5.1E-21	2.0E-13
Acenaphthene	Water	river	3.6E-12	1.2E-17	4.1E-19	7.1E-09
Acenaphthylene	Air		3.1E-13	1.3E-19	0.0E+00	0.0E+00
Acenaphthylene	Water	ocean	1.3E-14	8.3E-21	0.0E+00	0.0E+00
Acenaphthylene	Water	river	2.2E-13	6.6E-19	0.0E+00	0.0E+00
Acephate	Air	low. pop.	5.3E-12	5.9E-19	1.6E-15	1.5E-10
Acephate	Soil	agricultural	4.9E-10	1.8E-17	5.0E-14	2.2E-08
Acetaldehyde	Air		1.8E-08	1.7E-15	8.9E-15	5.6E-09
Acetaldehyde	Air	high. pop.	6.7E-08	1.2E-14	6.2E-14	2.0E-08
Acetaldehyde	Air	low. pop.	3.2E-09	2.7E-17	1.4E-16	1.0E-09
Acetaldehyde	Water	river	1.6E-07	8.1E-15	4.1E-14	4.0E-06
Acetamide	Air	low. pop.	1.3E-12	6.9E-19	0.0E+00	7.6E-13
Acetamide	Soil	agricultural	7.1E-11	2.0E-17	0.0E+00	6.3E-11
Acetic acid	Air		2.2E-07	0.0E+00	0.0E+00	5.9E-07
Acetic acid	Air	high. pop.	3.1E-07	0.0E+00	0.0E+00	9.1E-07
Acetic acid	Air	low. pop.	4.6E-08	0.0E+00	0.0E+00	1.0E-07
Acetic acid	Water	river	1.7E-06	0.0E+00	0.0E+00	8.7E-05
Acetochlor	Soil	agricultural	1.0E-09	0.0E+00	0.0E+00	1.0E-06
Acetone	Air		2.9E-09	0.0E+00	1.4E-17	1.5E-10
Acetone	Air	high. pop.	4.5E-08	0.0E+00	3.8E-16	2.4E-09
Acetone	Air	low. pop.	5.5E-08	0.0E+00	8.7E-17	2.9E-09
Acetone	Water		8.0E-11	0.0E+00	2.9E-19	5.8E-11
Acetone	Water	river	2.2E-08	0.0E+00	8.2E-17	1.6E-08
Acetonitrile	Air	low. pop.	5.0E-10	0.0E+00	8.0E-18	2.3E-10
Acetonitrile	Water	river	1.1E-12	0.0E+00	3.7E-20	6.3E-12
Acetyl chloride	Water	river	2.0E-12	0.0E+00	0.0E+00	1.4E-10
Acifluorfen	Air	low. pop.	7.3E-13	3.1E-18	0.0E+00	0.0E+00
Acifluorfen	Soil	agricultural	3.1E-14	1.6E-19	0.0E+00	0.0E+00
Aclonifen	Soil	agricultural	5.8E-06	0.0E+00	0.0E+00	3.5E-02
Acrolein	Air		3.8E-09	0.0E+00	2.7E-12	4.2E-07
Acrolein	Air	high. pop.	5.9E-11	0.0E+00	8.2E-14	6.5E-09
Acrolein	Air	low. pop.	1.9E-09	0.0E+00	9.7E-14	2.2E-07
Acrylic acid	Air	high. pop.	9.2E-13	0.0E+00	8.7E-17	1.2E-11
Alachlor	Air	low. pop.	5.1E-12	0.0E+00	0.0E+00	4.2E-09
Alachlor	Soil	agricultural	1.6E-10	0.0E+00	0.0E+00	2.2E-07

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Aldicarb	Soil	agricultural	1.3E-09	0.0E+00	5.4E-15	8.1E-07
Aldrin	Soil	agricultural	8.0E-09	5.5E-13	1.7E-12	3.0E-06
Allyl chloride	Water		1.1E-10	0.0E+00	4.3E-17	6.6E-09
Alpha-cypermethrin	Soil	agricultural	2.5E-12	0.0E+00	1.7E-19	1.2E-08
Ametryn	Soil	agricultural	5.1E-11	0.0E+00	0.0E+00	9.1E-08
Amitraz	Soil	agricultural	6.7E-11	0.0E+00	3.4E-18	9.4E-12
Aniline	Air	high. pop.	2.9E-11	1.0E-18	5.1E-17	1.2E-10
Aniline	Water	river	7.0E-11	4.4E-18	2.2E-16	4.1E-08
Anthranilic acid	Air	high. pop.	1.2E-12	0.0E+00	0.0E+00	0.0E+00
Anthraquinone	Soil	agricultural	1.5E-11	0.0E+00	0.0E+00	4.9E-11
Asulam	Soil	agricultural	1.3E-12	0.0E+00	1.3E-19	1.5E-11
Atrazine	Air	low. pop.	4.4E-12	8.4E-18	9.8E-18	7.7E-09
Atrazine	Water	groundwater	2.0E-12	7.4E-18	8.6E-18	6.9E-09
Atrazine	Water	river	7.7E-15	2.9E-20	3.3E-20	6.8E-10
Atrazine	Soil	agricultural	4.2E-09	3.4E-15	3.9E-15	1.5E-05
Azinphos-methyl	Soil	agricultural	2.8E-12	0.0E+00	6.4E-18	2.0E-08
Azoxystrobin	Air	low. pop.	2.4E-12	0.0E+00	0.0E+00	2.9E-08
Azoxystrobin	Soil	agricultural	3.2E-11	0.0E+00	0.0E+00	5.0E-07
Benfluralin	Soil	agricultural	3.4E-10	0.0E+00	1.7E-17	3.7E-09
Benomyl	Soil	agricultural	7.8E-13	0.0E+00	2.8E-20	6.2E-10
Bentazone	Air	low. pop.	2.2E-12	0.0E+00	9.3E-19	7.3E-12
Bentazone	Water	groundwater	7.3E-14	0.0E+00	8.9E-20	1.1E-12
Bentazone	Water	river	4.5E-17	0.0E+00	5.5E-23	9.1E-15
Bentazone	Soil	agricultural	4.4E-12	0.0E+00	2.3E-18	6.7E-11
Benzaldehyde	Air		2.9E-09	5.1E-17	6.7E-17	9.8E-09
Benzaldehyde	Air	high. pop.	2.9E-11	9.7E-19	1.3E-18	9.8E-11
Benzaldehyde	Air	low. pop.	5.2E-10	1.1E-18	1.4E-18	1.8E-09
Benzene	Air		2.5E-07	6.4E-14	1.6E-14	1.3E-08
Benzene	Air	high. pop.	3.4E-07	1.5E-13	3.8E-14	1.8E-08
Benzene	Air	low. pop.	1.5E-06	1.3E-13	3.3E-14	8.2E-08
Benzene	Air	stratosphere + troposphere	3.4E-13	2.8E-20	7.2E-21	1.8E-14
Benzene	Water		1.3E-08	1.8E-15	4.5E-16	3.4E-07
Benzene	Water	ocean	5.8E-09	2.1E-16	5.2E-17	1.3E-10
Benzene	Water	river	4.9E-07	6.5E-14	1.6E-14	1.2E-05
Benzene, 1-methyl-2-nitro-	Air	high. pop.	1.4E-12	1.1E-17	0.0E+00	2.9E-11
Benzene, 1,2-dichloro-	Air	high. pop.	8.1E-12	0.0E+00	4.2E-19	1.8E-11

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Benzene, 1,2-dichloro-	Water	river	2.2E-07	0.0E+00	7.3E-15	5.0E-05
Benzene, chloro-	Water	river	3.1E-07	1.6E-14	1.6E-14	5.1E-05
Benzene, ethyl-	Air		3.0E-13	9.7E-20	1.6E-21	8.2E-15
Benzene, ethyl-	Air	high. pop.	1.7E-08	1.0E-14	1.7E-16	4.8E-10
Benzene, ethyl-	Air	low. pop.	6.5E-10	3.0E-17	5.3E-19	1.8E-11
Benzene, ethyl-	Water		7.5E-10	3.3E-17	1.1E-17	5.4E-08
Benzene, ethyl-	Water	ocean	8.0E-10	8.2E-18	1.0E-18	4.8E-12
Benzene, ethyl-	Water	river	1.4E-08	6.0E-16	2.1E-16	9.8E-07
Benzene, hexachloro-	Air		2.1E-11	1.5E-15	5.1E-16	1.1E-08
Benzene, hexachloro-	Air	high. pop.	4.7E-14	3.5E-18	1.2E-18	2.5E-11
Benzene, hexachloro-	Air	low. pop.	3.4E-20	2.3E-24	8.0E-25	1.8E-17
Benzene, pentachloro-	Air	high. pop.	1.2E-13	0.0E+00	3.2E-18	3.3E-11
Benzene, pentachloronitro-	Soil	agricultural	2.9E-11	7.4E-17	3.3E-16	1.1E-08
Benzo(a)anthracene	Air		5.9E-15	2.3E-18	0.0E+00	4.7E-11
Benzo(a)pyrene	Air		5.2E-11	2.1E-13	0.0E+00	8.1E-09
Benzo(a)pyrene	Air	high. pop.	1.6E-10	7.2E-13	0.0E+00	3.6E-08
Benzo(a)pyrene	Air	low. pop.	9.9E-09	3.6E-11	0.0E+00	8.5E-07
Benzo(b)fluoranthene	Air		7.0E-15	6.7E-18	0.0E+00	0.0E+00
Benzo(g,h,i)perylene	Air		4.3E-16	1.4E-20	0.0E+00	0.0E+00
Benzo(k)fluoranthene	Air		5.0E-15	2.2E-18	0.0E+00	0.0E+00
Bifenoxy	Soil	agricultural	4.0E-12	0.0E+00	0.0E+00	4.2E-10
Bifenthrin	Soil	agricultural	3.8E-12	0.0E+00	5.1E-19	5.2E-09
Bitertanol	Soil	agricultural	1.6E-12	0.0E+00	1.5E-18	8.9E-11
Bromacil	Soil	agricultural	5.1E-10	0.0E+00	0.0E+00	4.0E-07
Bromoxynil	Air	low. pop.	4.9E-14	0.0E+00	4.4E-20	3.3E-11
Bromoxynil	Water	groundwater	2.9E-13	0.0E+00	9.3E-19	5.6E-11
Bromoxynil	Water	river	1.2E-15	0.0E+00	3.8E-21	1.9E-11
Bromoxynil	Soil	agricultural	3.1E-11	0.0E+00	1.4E-17	6.1E-09
Bromuconazole	Soil	agricultural	1.8E-14	0.0E+00	0.0E+00	7.2E-11
Butadiene	Air		7.5E-13	4.3E-19	6.4E-19	0.0E+00
Butadiene	Air	high. pop.	4.2E-13	4.8E-19	7.1E-19	0.0E+00
Butadiene	Air	low. pop.	8.7E-14	1.4E-21	2.1E-21	0.0E+00

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Butadiene	Air	stratosphere + troposphere	3.2E-13	5.2E-21	7.8E-21	0.0E+00
Butyl acetate	Water	river	6.4E-09	0.0E+00	0.0E+00	9.0E-08
Butyric acid, 4-(2,4-dichlorophenoxy)-	Air	low. pop.	2.5E-13	0.0E+00	2.3E-19	8.4E-12
Butyric acid, 4-(2,4-dichlorophenoxy)-	Soil	agricultural	4.2E-12	0.0E+00	2.5E-18	1.4E-10
Butyrolactone	Air	high. pop.	2.0E-12	0.0E+00	0.0E+00	6.5E-11
Butyrolactone	Water	river	4.7E-12	0.0E+00	0.0E+00	7.3E-10
Captan	Soil	agricultural	1.5E-09	5.2E-18	5.5E-17	5.9E-07
Carbaryl	Air	low. pop.	6.2E-13	1.0E-18	7.5E-19	4.5E-10
Carbaryl	Water	groundwater	2.3E-16	1.6E-21	1.2E-21	1.7E-13
Carbaryl	Water	river	2.9E-18	2.0E-23	1.5E-23	1.3E-13
Carbaryl	Soil	agricultural	9.9E-12	5.5E-18	4.1E-18	7.2E-09
Carbendazim	Soil	agricultural	1.5E-09	0.0E+00	1.8E-16	2.6E-05
Carbetamide	Soil	agricultural	3.4E-08	0.0E+00	0.0E+00	1.4E-06
Carbofuran	Soil	agricultural	4.6E-10	0.0E+00	4.2E-15	2.7E-06
Carbon disulfide	Air		1.3E-15	0.0E+00	7.0E-21	1.0E-16
Carbon disulfide	Air	high. pop.	6.2E-10	0.0E+00	5.2E-15	4.6E-11
Carbon disulfide	Air	low. pop.	5.8E-07	0.0E+00	1.2E-12	4.3E-08
Carbon disulfide	Water	river	1.1E-07	0.0E+00	2.1E-13	6.8E-06
Carfentrazone-ethyl	Air	low. pop.	6.7E-14	0.0E+00	0.0E+00	3.7E-10
Carfentrazone-ethyl	Soil	agricultural	1.5E-13	0.0E+00	0.0E+00	7.1E-12
Chloramine	Air	high. pop.	2.0E-09	0.0E+00	4.1E-15	2.5E-05
Chloramine	Water	river	1.8E-08	0.0E+00	9.5E-15	1.3E-03
Chlorfenvinphos	Soil	agricultural	2.1E-11	0.0E+00	4.5E-15	1.1E-07
Chloridazon	Soil	agricultural	1.6E-12	0.0E+00	0.0E+00	9.5E-10
Chlormequat	Soil	agricultural	1.4E-05	0.0E+00	5.9E-12	0.0E+00
Chloroacetic acid	Air	high. pop.	9.4E-08	0.0E+00	0.0E+00	3.5E-05
Chloroacetic acid	Water	river	3.1E-06	0.0E+00	0.0E+00	9.0E-03
Chloroform	Air		6.1E-16	1.2E-22	6.8E-22	1.5E-16
Chloroform	Air	high. pop.	7.8E-10	2.1E-16	1.2E-15	1.9E-10
Chloroform	Air	low. pop.	6.0E-10	7.7E-17	4.4E-16	1.5E-10
Chloroform	Water	river	2.5E-12	5.4E-19	2.1E-18	4.0E-11
Chlorosulfonic acid	Air		1.9E-14	0.0E+00	0.0E+00	1.5E-12
Chlorosulfonic acid	Air	high. pop.	1.6E-12	0.0E+00	0.0E+00	1.3E-10
Chlorosulfonic acid	Water	river	3.9E-12	0.0E+00	0.0E+00	2.3E-09
Chlorothalonil	Soil	agricultural	1.0E-05	4.3E-14	1.3E-12	7.3E-02
Chlorpyrifos	Air	low. pop.	2.4E-11	0.0E+00	8.0E-17	2.7E-07

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Chlorpyrifos	Soil	agricultural	1.2E-09	0.0E+00	8.9E-15	6.4E-06
Chlorsulfuron	Soil	agricultural	2.5E-14	0.0E+00	2.3E-20	3.5E-11
Chlortoluron	Soil	agricultural	8.2E-06	0.0E+00	0.0E+00	1.5E-03
Choline chloride	Soil	agricultural	3.4E-12	0.0E+00	0.0E+00	8.3E-12
Chrysene	Air		6.4E-16	3.1E-20	0.0E+00	0.0E+00
Clethodim	Air	low. pop.	3.6E-12	0.0E+00	0.0E+00	4.9E-11
Clethodim	Soil	agricultural	8.1E-12	0.0E+00	0.0E+00	1.7E-11
Clodinafop-propargyl	Soil	agricultural	3.7E-13	0.0E+00	0.0E+00	1.2E-12
Clomazone	Soil	agricultural	8.7E-10	0.0E+00	0.0E+00	2.5E-07
Clopyralid	Soil	agricultural	2.1E-11	0.0E+00	0.0E+00	9.4E-10
Cloquintocet-mexyl	Soil	agricultural	8.9E-14	0.0E+00	0.0E+00	4.6E-13
Cumene	Air		5.5E-17	0.0E+00	5.9E-25	4.3E-18
Cumene	Air	high. pop.	3.0E-08	0.0E+00	6.0E-16	2.5E-09
Cumene	Air	low. pop.	3.4E-11	0.0E+00	5.8E-20	2.5E-12
Cumene	Water	river	7.3E-08	0.0E+00	8.7E-16	2.0E-05
Cyclohexane	Air	high. pop.	3.7E-12	0.0E+00	7.8E-20	2.1E-15
Cycloxydim	Soil	agricultural	1.9E-15	0.0E+00	0.0E+00	7.9E-16
Cyfluthrin	Air	low. pop.	1.3E-13	0.0E+00	2.1E-19	1.1E-06
Cyfluthrin	Soil	agricultural	6.0E-12	0.0E+00	3.0E-19	1.5E-07
Cymoxanil	Soil	agricultural	7.4E-11	0.0E+00	0.0E+00	5.7E-09
Cypermethrin	Air	low. pop.	3.1E-13	0.0E+00	3.0E-19	1.5E-07
Cypermethrin	Soil	agricultural	1.8E-09	0.0E+00	2.3E-16	2.4E-05
Cyproconazole	Soil	agricultural	1.5E-12	0.0E+00	0.0E+00	3.5E-10
Cyprodinil	Soil	agricultural	2.0E-10	0.0E+00	0.0E+00	4.4E-08
Deltamethrin	Soil	agricultural	3.7E-11	0.0E+00	7.6E-18	2.7E-08
Diazinon	Soil	agricultural	2.4E-10	0.0E+00	7.5E-15	3.8E-07
Dibenz(a,h)anthracene	Air		3.3E-15	1.8E-17	0.0E+00	2.5E-13
Dicamba	Air	low. pop.	1.3E-12	0.0E+00	2.1E-18	9.3E-11
Dicamba	Water	groundwater	2.1E-13	0.0E+00	4.9E-19	5.9E-12
Dicamba	Water	river	8.5E-16	0.0E+00	2.0E-21	1.6E-12
Dicamba	Soil	agricultural	4.3E-11	0.0E+00	6.5E-18	1.2E-09
Dichlorprop	Air	low. pop.	5.9E-14	0.0E+00	0.0E+00	7.0E-13
Dichlorprop	Water	groundwater	6.1E-14	0.0E+00	0.0E+00	6.8E-13
Dichlorprop	Water	river	2.6E-16	0.0E+00	0.0E+00	1.1E-13
Dichlorprop	Soil	agricultural	2.5E-12	0.0E+00	0.0E+00	2.7E-11
Diclofop-methyl	Soil	agricultural	2.4E-11	0.0E+00	0.0E+00	9.9E-10

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Dicrotophos	Soil	agricultural	7.0E-11	0.0E+00	1.6E-15	1.0E-07
Diethyl ether	Air	high. pop.	2.5E-14	0.0E+00	3.1E-22	4.6E-17
Diethylamine	Air	high. pop.	2.7E-09	0.0E+00	0.0E+00	5.9E-09
Diethylamine	Water	river	6.6E-09	0.0E+00	0.0E+00	7.2E-07
Diethylene glycol	Air	high. pop.	2.8E-13	1.3E-20	0.0E+00	1.5E-14
Difenoconazole	Soil	agricultural	3.5E-10	0.0E+00	0.0E+00	5.2E-07
Diflubenzuron	Air	low. pop.	6.7E-14	0.0E+00	8.1E-20	1.2E-08
Diflubenzuron	Soil	agricultural	3.1E-09	0.0E+00	3.0E-17	4.5E-06
Diflufenican	Soil	agricultural	6.6E-11	0.0E+00	0.0E+00	1.6E-09
Dimethachlor	Soil	agricultural	2.1E-09	0.0E+00	0.0E+00	2.8E-07
Dimethenamid	Air	low. pop.	5.8E-14	0.0E+00	0.0E+00	8.8E-11
Dimethenamid	Water	groundwater	2.0E-14	0.0E+00	0.0E+00	1.2E-10
Dimethenamid	Water	river	2.6E-16	0.0E+00	0.0E+00	3.6E-11
Dimethenamid	Soil	agricultural	5.5E-06	0.0E+00	0.0E+00	3.1E-02
Dimethoate	Soil	agricultural	1.5E-10	0.0E+00	1.9E-16	1.9E-07
Dimethomorph	Soil	agricultural	5.6E-11	0.0E+00	0.0E+00	8.3E-09
Dimethyl malonate	Air	high. pop.	1.6E-12	0.0E+00	0.0E+00	2.7E-11
Dimethylamine	Air	high. pop.	2.1E-13	0.0E+00	0.0E+00	7.7E-13
Dimethylamine	Water	river	1.4E-08	0.0E+00	0.0E+00	2.3E-06
Dioxin, 2,3,7,8 Tetrachlorodibenzo- p-	Air		6.1E-14	2.3E-12	0.0E+00	1.9E-08
Dioxin, 2,3,7,8 Tetrachlorodibenzo- p-	Air	high. pop.	8.6E-15	3.4E-13	0.0E+00	2.9E-09
Dioxin, 2,3,7,8 Tetrachlorodibenzo- p-	Air	low. pop.	1.4E-14	5.4E-13	0.0E+00	4.2E-09
Dioxin, 2,3,7,8 Tetrachlorodibenzo- p-	Air	low. pop., long-term	4.6E-19	1.7E-17	0.0E+00	1.4E-13
Dipropylamine	Air	high. pop.	8.0E-12	0.0E+00	0.0E+00	1.1E-10
Dipropylamine	Water	river	1.9E-11	0.0E+00	0.0E+00	1.3E-08
Dipropylthiocarbami c acid S-ethyl ester	Soil	agricultural	1.1E-10	0.0E+00	1.1E-16	2.2E-09
Diquat	Soil	agricultural	2.2E-11	0.0E+00	4.6E-16	1.1E-07
Diquat dibromide	Soil	agricultural	2.9E-11	0.0E+00	1.2E-15	2.2E-06
Dithianone	Soil	agricultural	2.2E-10	0.0E+00	2.6E-16	3.2E-07
Diuron	Soil	agricultural	1.0E-09	0.0E+00	3.8E-15	4.7E-06
Endosulfan	Soil	agricultural	6.4E-10	0.0E+00	8.2E-16	5.2E-07

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Endothall	Soil	agricultural	2.2E-11	0.0E+00	5.1E-18	3.2E-10
Epoxiconazole	Soil	agricultural	4.1E-12	0.0E+00	0.0E+00	4.4E-09
Esfenvalerate	Air	low. pop.	7.6E-13	0.0E+00	0.0E+00	2.0E-07
Esfenvalerate	Soil	agricultural	1.6E-12	0.0E+00	0.0E+00	6.6E-08
Ethalfuralin	Soil	agricultural	7.1E-10	0.0E+00	0.0E+00	2.7E-07
Ethane, 1,1,1-trichloro-, HCFC-140	Air		1.1E-15	0.0E+00	1.8E-23	2.1E-16
Ethane, 1,1,1-trichloro-, HCFC-140	Air	low. pop.	1.2E-10	0.0E+00	1.8E-18	2.3E-11
Ethane, 1,1,1-trichloro-, HCFC-140	Water	river	6.6E-17	0.0E+00	9.9E-25	5.5E-16
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	Air		1.3E-09	1.5E-17	5.4E-18	0.0E+00
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	Air	high. pop.	1.7E-10	2.1E-18	7.6E-19	0.0E+00
Ethane, 1,1,1,2-tetrafluoro-, HFC-134a	Air	low. pop.	4.4E-10	4.9E-18	1.8E-18	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air		2.1E-10	0.0E+00	7.7E-19	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air	high. pop.	4.4E-14	0.0E+00	2.2E-22	0.0E+00
Ethane, 1,1,2-trichloro-1,2,2-trifluoro-, CFC-113	Air	low. pop., long-term	2.4E-11	0.0E+00	5.6E-20	0.0E+00
Ethane, 1,2-dichloro-	Air		1.8E-14	6.3E-21	0.0E+00	2.3E-15
Ethane, 1,2-dichloro-	Air	high. pop.	9.5E-08	4.9E-14	0.0E+00	1.2E-08
Ethane, 1,2-dichloro-	Air	low. pop.	2.5E-10	4.2E-17	0.0E+00	3.0E-11
Ethane, 1,2-dichloro-	Water	river	1.0E-07	7.3E-14	0.0E+00	6.1E-07
Ethane, 2-chloro-1,1,1,2-tetrafluoro-, HCFC-124	Air		2.1E-10	0.0E+00	0.0E+00	0.0E+00
Ethanol	Air		1.5E-12	3.0E-21	0.0E+00	2.2E-13
Ethanol	Air	high. pop.	5.5E-08	2.0E-16	0.0E+00	8.5E-09
Ethanol	Air	low. pop.	1.2E-08	7.0E-18	0.0E+00	1.9E-09
Ethanol	Water		2.9E-14	6.5E-23	0.0E+00	7.8E-14
Ethanol	Water	river	1.3E-08	2.9E-17	0.0E+00	3.5E-08

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Ethene, chloro-	Air		4.1E-16	1.1E-21	3.8E-22	0.0E+00
Ethene, chloro-	Air	high. pop.	3.3E-08	1.7E-13	5.7E-14	0.0E+00
Ethene, chloro-	Water	river	3.9E-10	3.3E-16	1.0E-15	0.0E+00
Ethene, tetrachloro-	Air		9.0E-13	2.5E-19	9.5E-19	5.8E-13
Ethene, tetrachloro-	Air	high. pop.	1.3E-10	5.0E-17	1.9E-16	8.5E-11
Ethene, tetrachloro-	Air	low. pop.	2.7E-10	4.7E-17	1.8E-16	1.7E-10
Ethephon	Air	low. pop.	2.2E-18	0.0E+00	2.0E-23	2.4E-16
Ethephon	Water	groundwater	1.5E-19	0.0E+00	7.5E-25	1.5E-17
Ethephon	Water	river	8.9E-22	0.0E+00	4.5E-27	1.2E-18
Ethephon	Soil	agricultural	2.3E-10	0.0E+00	2.2E-16	2.4E-08
Ethofumesate	Soil	agricultural	5.9E-10	0.0E+00	0.0E+00	9.2E-08
Ethoprop	Soil	agricultural	2.7E-11	0.0E+00	1.1E-14	3.7E-07
Ethyl acetate	Air	high. pop.	4.5E-08	0.0E+00	3.6E-16	4.1E-09
Ethyl acetate	Water	river	1.2E-10	0.0E+00	3.1E-19	3.6E-10
Ethylamine	Air	high. pop.	6.7E-12	0.0E+00	0.0E+00	9.7E-12
Ethylamine	Water	river	1.6E-11	0.0E+00	0.0E+00	8.4E-10
Ethylene diamine	Air	high. pop.	1.8E-08	0.0E+00	0.0E+00	1.7E-07
Ethylene diamine	Water	river	4.4E-08	0.0E+00	0.0E+00	1.7E-05
Ethylene oxide	Air		7.4E-12	4.7E-18	0.0E+00	4.8E-12
Ethylene oxide	Air	high. pop.	1.5E-10	1.5E-16	0.0E+00	9.5E-11
Ethylene oxide	Air	low. pop.	8.4E-13	2.1E-19	0.0E+00	5.5E-13
Ethylene oxide	Air	stratosphere + troposphere	3.1E-12	7.7E-19	0.0E+00	2.0E-12
Ethylene oxide	Water	river	3.3E-08	2.9E-14	0.0E+00	3.7E-07
Fenamiphos	Soil	agricultural	2.8E-10	0.0E+00	2.8E-16	2.1E-07
Fenbuconazole	Soil	agricultural	1.3E-13	0.0E+00	1.5E-19	3.1E-10
Fenoxaprop-P ethyl ester	Soil	agricultural	1.1E-12	0.0E+00	0.0E+00	5.5E-13
Fenoxaprop ethyl ester	Soil	agricultural	2.0E-12	0.0E+00	0.0E+00	1.1E-11
Fenoxycarb	Soil	agricultural	1.6E-11	0.0E+00	0.0E+00	8.2E-10
Fenpiclonil	Soil	agricultural	1.8E-11	0.0E+00	0.0E+00	4.3E-08
Fentin hydroxide	Soil	agricultural	4.6E-12	0.0E+00	2.5E-16	5.6E-06
Fipronil	Soil	agricultural	4.2E-10	0.0E+00	9.8E-15	7.2E-06
Fluazifop-p-butyl	Air	low. pop.	1.4E-12	0.0E+00	0.0E+00	3.4E-10
Fludioxonil	Soil	agricultural	3.4E-11	0.0E+00	0.0E+00	8.6E-09
Flufenacet	Air	low. pop.	5.3E-13	0.0E+00	0.0E+00	1.8E-09
Flufenacet	Soil	agricultural	1.6E-11	0.0E+00	0.0E+00	5.7E-08
Flumetsulam	Air	low. pop.	1.3E-13	0.0E+00	0.0E+00	3.5E-10

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Flumetsulam	Soil	agricultural	5.9E-12	0.0E+00	0.0E+00	1.8E-08
Flumiclorac-pentyl	Air	low. pop.	2.1E-13	0.0E+00	0.0E+00	1.5E-10
Flumiclorac-pentyl	Soil	agricultural	9.2E-15	0.0E+00	0.0E+00	8.7E-14
Flumioxazin	Air	low. pop.	2.2E-12	0.0E+00	0.0E+00	5.3E-09
Flumioxazin	Soil	agricultural	2.8E-12	0.0E+00	0.0E+00	4.0E-08
Fluoranthene	Air		5.4E-14	2.9E-19	1.4E-20	3.6E-11
Fluorene	Air		4.9E-14	7.6E-20	3.7E-21	7.6E-13
Fluroxypyr	Soil	agricultural	1.9E-12	0.0E+00	0.0E+00	9.0E-10
Flutolanil	Soil	agricultural	5.2E-12	0.0E+00	4.6E-18	1.8E-09
Folpet	Soil	agricultural	1.2E-05	3.7E-14	1.3E-13	3.9E-02
Fomesafen	Air	low. pop.	8.0E-12	9.9E-17	0.0E+00	4.4E-10
Fomesafen	Soil	agricultural	1.8E-11	2.2E-16	0.0E+00	1.3E-09
Formaldehyde	Air		4.6E-08	6.0E-13	7.7E-15	7.7E-07
Formaldehyde	Air	high. pop.	1.7E-07	4.3E-12	4.5E-14	3.1E-06
Formaldehyde	Air	low. pop.	9.3E-08	1.1E-13	6.8E-15	1.5E-06
Formaldehyde	Air	stratosphere + troposphere	2.7E-12	3.1E-18	2.0E-19	4.2E-11
Formaldehyde	Water		8.5E-09	1.2E-15	2.7E-15	2.5E-06
Formaldehyde	Water	river	1.4E-07	1.9E-14	4.3E-14	3.9E-05
Formamide	Air	high. pop.	2.0E-12	0.0E+00	0.0E+00	3.0E-12
Formamide	Water	river	4.7E-12	0.0E+00	0.0E+00	3.3E-11
Formic acid	Air	high. pop.	5.3E-11	0.0E+00	0.0E+00	1.5E-10
Formic acid	Air	low. pop.	3.1E-09	0.0E+00	0.0E+00	6.7E-09
Formic acid	Water	river	1.4E-12	0.0E+00	0.0E+00	6.2E-11
Fosetyl-aluminium	Soil	agricultural	1.3E-09	9.8E-20	5.7E-20	2.8E-09
Furan	Air		8.8E-17	2.8E-21	3.2E-22	2.2E-19
Furan	Air	low. pop.	1.3E-08	1.8E-14	2.0E-15	3.5E-11
Glufosinate ammonium	Soil	agricultural	6.1E-11	0.0E+00	3.5E-18	2.5E-10
Glutaraldehyde	Water	ocean	1.8E-10	0.0E+00	0.0E+00	1.7E-11
Glyphosate	Air	low. pop.	1.6E-09	0.0E+00	6.4E-17	1.6E-08
Glyphosate	Water	groundwater	5.0E-12	0.0E+00	8.0E-19	3.6E-10
Glyphosate	Water	river	2.6E-14	0.0E+00	4.1E-21	8.3E-12
Glyphosate	Soil	agricultural	6.7E-05	0.0E+00	7.8E-12	4.8E-03
Glyphosate	Soil	industrial	2.0E-09	0.0E+00	7.0E-17	1.4E-07
Heptane	Air		6.3E-10	0.0E+00	0.0E+00	9.2E-15
Heptane	Air	high. pop.	1.6E-07	0.0E+00	0.0E+00	4.0E-12
Hexane	Air		7.0E-16	6.7E-25	9.1E-23	9.4E-20

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Hexane	Air	high. pop.	4.1E-07	7.2E-16	9.8E-14	8.6E-11
Hexane	Air	low. pop.	2.7E-07	4.2E-17	5.8E-15	1.6E-11
Hexazinone	Soil	agricultural	4.7E-11	0.0E+00	4.6E-17	1.2E-06
Hydramethylnon	Soil	agricultural	1.1E-12	0.0E+00	9.4E-19	2.0E-12
Imazamox	Air	low. pop.	3.2E-13	0.0E+00	0.0E+00	1.5E-10
Imazamox	Soil	agricultural	2.4E-12	0.0E+00	0.0E+00	1.3E-09
Imazapyr	Soil	agricultural	8.4E-14	0.0E+00	0.0E+00	6.9E-14
Imazethapyr	Air	low. pop.	2.1E-12	0.0E+00	4.9E-19	2.5E-10
Imazethapyr	Soil	agricultural	6.3E-12	0.0E+00	9.5E-19	9.7E-10
Imidacloprid	Soil	agricultural	2.6E-06	0.0E+00	5.2E-12	3.2E-03
Indeno(1,2,3-cd)pyrene	Air		1.3E-15	5.4E-19	0.0E+00	0.0E+00
Ioxynil	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	1.5E-08
Iprodione	Soil	agricultural	1.4E-09	0.0E+00	1.4E-15	3.3E-06
Isoprene	Air		1.2E-15	8.1E-23	0.0E+00	5.3E-20
Isoprene	Air	low. pop.	4.5E-11	6.4E-20	0.0E+00	1.5E-15
Isopropylamine	Air	high. pop.	3.3E-12	0.0E+00	0.0E+00	1.3E-11
Isopropylamine	Water	river	8.0E-12	0.0E+00	0.0E+00	1.3E-09
Isoproturon	Soil	agricultural	1.2E-05	0.0E+00	0.0E+00	1.5E-02
Isoxaflutole	Soil	agricultural	1.0E-11	0.0E+00	0.0E+00	1.7E-09
Kresoxim-methyl	Soil	agricultural	9.9E-13	0.0E+00	3.2E-20	9.5E-10
Lambda-cyhalothrin	Air	low. pop.	7.0E-20	0.0E+00	0.0E+00	5.9E-14
Lambda-cyhalothrin	Water	groundwater	3.6E-23	0.0E+00	0.0E+00	3.3E-19
Lambda-cyhalothrin	Water	river	8.9E-26	0.0E+00	0.0E+00	1.2E-17
Lambda-cyhalothrin	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	9.7E-07
Lenacil	Soil	agricultural	2.4E-11	0.0E+00	0.0E+00	9.3E-08
Linuron	Soil	agricultural	2.9E-09	0.0E+00	2.4E-14	1.4E-05
m-Xylene	Air		2.1E-09	0.0E+00	0.0E+00	3.8E-11
m-Xylene	Air	high. pop.	1.5E-08	0.0E+00	0.0E+00	2.8E-10
m-Xylene	Air	low. pop.	9.4E-13	0.0E+00	0.0E+00	1.7E-14
m-Xylene	Water		2.4E-10	0.0E+00	0.0E+00	2.9E-08
m-Xylene	Water	river	2.3E-08	0.0E+00	0.0E+00	2.7E-06
Malathion	Soil	agricultural	4.1E-11	0.0E+00	7.5E-20	2.8E-09
Maleic hydrazide	Soil	agricultural	2.9E-11	0.0E+00	4.1E-19	3.0E-10
Mancozeb	Soil	agricultural	3.5E-05	0.0E+00	7.3E-12	6.9E-02
Maneb	Soil	agricultural	6.7E-13	1.6E-20	5.5E-20	7.1E-10
Mcpa - sodium salt	Soil	agricultural	5.3E-06	0.0E+00	0.0E+00	1.7E-04
MCPB	Air	low. pop.	8.1E-14	0.0E+00	4.7E-20	2.7E-12

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
MCPB	Water	groundwater	8.6E-16	0.0E+00	1.5E-21	2.0E-14
MCPB	Water	river	1.9E-13	0.0E+00	3.2E-19	3.6E-10
MCPB	Soil	agricultural	2.1E-11	0.0E+00	3.6E-18	4.8E-10
Mepiquat chloride	Soil	agricultural	2.5E-11	0.0E+00	7.8E-23	7.4E-13
Metalaxil	Soil	agricultural	1.6E-11	0.0E+00	6.2E-18	2.8E-09
Metalaxyl-M	Soil	agricultural	2.1E-10	0.0E+00	0.0E+00	7.3E-08
Metam-sodium dihydrate	Soil	agricultural	1.7E-05	0.0E+00	0.0E+00	1.5E-01
Metamitron	Soil	agricultural	3.9E-06	0.0E+00	0.0E+00	3.6E-05
Metazachlor	Soil	agricultural	5.0E-06	0.0E+00	0.0E+00	2.1E-04
Methane, bromo-, Halon 1001	Air		1.7E-15	0.0E+00	1.4E-19	1.8E-14
Methane, chlorodifluoro-, HCFC-22	Air		1.3E-15	0.0E+00	1.1E-23	0.0E+00
Methane, chlorodifluoro-, HCFC-22	Air	high. pop.	1.9E-09	0.0E+00	1.7E-17	0.0E+00
Methane, chlorodifluoro-, HCFC-22	Air	low. pop.	4.6E-09	0.0E+00	3.7E-17	0.0E+00
Methane, dichloro-, HCC-30	Air		5.9E-11	3.3E-18	3.9E-17	4.9E-12
Methane, dichloro-, HCC-30	Air	high. pop.	4.1E-11	3.3E-18	3.8E-17	3.5E-12
Methane, dichloro-, HCC-30	Air	low. pop.	1.8E-09	6.0E-17	7.0E-16	1.5E-10
Methane, dichloro-, HCC-30	Water	river	9.0E-09	3.8E-16	4.2E-15	5.0E-08
Methane, dichlorodifluoro-, CFC-12	Air		1.1E-15	0.0E+00	2.5E-22	0.0E+00
Methane, dichlorodifluoro-, CFC-12	Air	high. pop.	4.8E-10	0.0E+00	1.6E-16	0.0E+00
Methane, dichlorodifluoro-, CFC-12	Air	low. pop.	2.4E-13	0.0E+00	2.9E-20	0.0E+00
Methane, monochloro-, R-40	Air	low. pop.	3.3E-09	0.0E+00	1.2E-15	1.9E-10
Methane, tetrachloro-, CFC-10	Air		4.9E-13	1.7E-18	5.7E-18	2.2E-14
Methane, tetrachloro-, CFC-10	Air	high. pop.	4.2E-10	2.0E-15	6.6E-15	1.8E-11

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Methane, trichlorofluoro-, CFC-11	Air	high. pop.	6.2E-13	0.0E+00	4.0E-20	0.0E+00
Methanol	Air		1.1E-07	0.0E+00	1.0E-15	2.1E-08
Methanol	Air	high. pop.	5.6E-07	0.0E+00	8.6E-15	1.1E-07
Methanol	Air	low. pop.	5.8E-08	0.0E+00	1.8E-16	1.1E-08
Methanol	Water		2.6E-09	0.0E+00	2.4E-17	5.9E-09
Methanol	Water	ocean	1.1E-09	0.0E+00	4.5E-20	2.6E-12
Methanol	Water	river	3.5E-08	0.0E+00	3.3E-16	8.0E-08
Methomyl	Air	low. pop.	7.6E-18	0.0E+00	5.3E-23	1.1E-14
Methomyl	Water	groundwater	1.2E-19	0.0E+00	1.4E-24	2.0E-16
Methomyl	Water	river	1.3E-21	0.0E+00	1.6E-26	3.8E-17
Methomyl	Soil	agricultural	2.4E-17	0.0E+00	6.7E-23	4.1E-14
Methoxyfenozide	Soil	agricultural	2.8E-11	0.0E+00	0.0E+00	2.7E-08
Methyl acetate	Air	high. pop.	1.5E-09	0.0E+00	0.0E+00	5.8E-10
Methyl acetate	Water	river	3.5E-09	0.0E+00	0.0E+00	2.7E-08
Methyl acrylate	Air	high. pop.	1.0E-12	0.0E+00	0.0E+00	2.8E-12
Methyl acrylate	Water	river	2.0E-11	0.0E+00	0.0E+00	6.4E-09
Methyl ethyl ketone	Air	high. pop.	4.5E-08	0.0E+00	5.1E-17	1.9E-09
Methyl ethyl ketone	Air	low. pop.	5.4E-13	0.0E+00	2.3E-22	2.3E-14
Methyl formate	Air	high. pop.	8.2E-13	0.0E+00	0.0E+00	3.1E-13
Methyl formate	Water	river	3.3E-13	0.0E+00	0.0E+00	2.7E-12
Methyl lactate	Air	high. pop.	6.9E-12	0.0E+00	0.0E+00	1.4E-11
Methylamine	Air	high. pop.	1.9E-12	0.0E+00	0.0E+00	4.9E-12
Methylamine	Water	river	4.6E-12	0.0E+00	0.0E+00	3.7E-10
Metiram	Soil	agricultural	7.8E-06	0.0E+00	9.8E-17	1.9E-07
Metolachlor	Air	low. pop.	1.7E-11	0.0E+00	4.6E-18	1.1E-08
Metolachlor	Water	groundwater	2.7E-13	0.0E+00	3.3E-19	3.3E-10
Metolachlor	Water	river	1.3E-15	0.0E+00	1.6E-21	8.5E-11
Metolachlor	Soil	agricultural	1.5E-05	0.0E+00	2.5E-12	1.8E-02
Metribuzin	Air	low. pop.	6.7E-12	0.0E+00	9.4E-18	2.2E-09
Metribuzin	Soil	agricultural	8.5E-11	0.0E+00	4.5E-17	5.9E-08
Metsulfuron-methyl	Soil	agricultural	3.6E-12	0.0E+00	2.8E-19	2.8E-09
Monocrotophos	Soil	agricultural	3.7E-10	0.0E+00	3.2E-14	2.9E-07
Monoethanolamine	Air	high. pop.	1.4E-08	0.0E+00	0.0E+00	2.3E-08
Monoethanolamine	Water		2.1E-11	0.0E+00	0.0E+00	1.3E-09
Monosodium acid methanearsonate	Soil	agricultural	3.6E-11	0.0E+00	0.0E+00	2.5E-09

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Napropamide	Soil	agricultural	4.6E-06	0.0E+00	9.3E-13	5.5E-04
Nicosulfuron	Soil	agricultural	4.6E-12	0.0E+00	0.0E+00	3.0E-10
Nitrobenzene	Air	high. pop.	4.1E-11	5.7E-17	2.8E-16	3.1E-10
Nitrobenzene	Water	river	1.6E-10	1.3E-16	6.3E-16	2.0E-08
o-Xylene	Air		8.3E-10	0.0E+00	0.0E+00	2.6E-11
o-Xylene	Air	high. pop.	6.6E-12	0.0E+00	0.0E+00	2.0E-13
o-Xylene	Water		1.8E-10	0.0E+00	0.0E+00	1.6E-08
Orbencarb	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	2.7E-08
Oryzalin	Soil	agricultural	4.5E-11	0.0E+00	4.3E-17	3.9E-07
Oxamyl	Soil	agricultural	2.2E-11	0.0E+00	2.5E-17	4.5E-08
Oxydemeton methyl	Soil	agricultural	5.4E-13	0.0E+00	0.0E+00	2.1E-10
Paraquat	Air	low. pop.	4.3E-12	0.0E+00	2.1E-17	1.2E-08
Paraquat	Soil	agricultural	2.4E-11	0.0E+00	1.3E-17	1.3E-07
Parathion	Soil	agricultural	7.6E-11	0.0E+00	2.1E-16	1.5E-06
Parathion, methyl	Air	low. pop.	8.2E-13	0.0E+00	2.3E-18	3.2E-10
Parathion, methyl	Soil	agricultural	3.5E-14	0.0E+00	3.5E-20	6.0E-12
Pendimethalin	Air	low. pop.	4.5E-11	0.0E+00	5.5E-18	1.5E-07
Pendimethalin	Water	groundwater	2.8E-14	0.0E+00	1.6E-20	5.8E-11
Pendimethalin	Water	river	4.7E-17	0.0E+00	2.6E-23	2.0E-11
Pendimethalin	Soil	agricultural	6.6E-06	0.0E+00	2.4E-12	1.4E-02
Pentane	Air		2.5E-10	0.0E+00	0.0E+00	2.3E-12
Pentane	Air	high. pop.	9.2E-07	0.0E+00	0.0E+00	1.1E-08
Pentane	Air	low. pop.	5.0E-07	0.0E+00	0.0E+00	2.9E-09
Permethrin	Air	low. pop.	6.7E-13	0.0E+00	2.9E-19	6.0E-09
Permethrin	Soil	agricultural	2.8E-12	0.0E+00	1.2E-19	7.5E-10
Phenanthrene	Air		7.5E-13	2.6E-18	0.0E+00	8.3E-11
Phenmedipham	Soil	agricultural	4.5E-10	0.0E+00	6.7E-18	2.7E-08
Phenol	Air		1.4E-10	0.0E+00	7.5E-18	3.1E-09
Phenol	Air	high. pop.	2.3E-08	0.0E+00	2.0E-15	5.9E-07
Phenol	Air	low. pop.	1.3E-09	0.0E+00	2.2E-17	2.4E-08
Phenol	Water		4.4E-09	0.0E+00	6.2E-16	4.1E-06
Phenol	Water	ocean	1.1E-08	0.0E+00	4.8E-18	2.2E-10
Phenol	Water	river	8.8E-08	0.0E+00	1.2E-14	8.1E-05
Phenol, 2,4-dichloro-	Air		1.1E-13	0.0E+00	2.1E-18	1.1E-10
Phenol, 2,4-dichloro-	Air	high. pop.	3.1E-12	0.0E+00	7.8E-17	3.2E-09
Phenol, pentachloro-	Air		3.5E-11	2.9E-16	6.3E-16	2.0E-07
Phenol, pentachloro-	Air	high. pop.	3.6E-13	3.0E-18	6.6E-18	2.2E-09

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Phenol, pentachloro-	Air	low. pop.	4.3E-09	3.5E-14	7.6E-14	2.1E-05
Phenol, pentachloro-	Soil		1.2E-12	8.5E-19	1.9E-18	3.5E-09
Phorate	Soil	agricultural	4.8E-11	0.0E+00	2.4E-15	5.0E-07
Phosmet	Soil	agricultural	5.3E-12	0.0E+00	2.6E-18	5.7E-08
Picloram	Soil	agricultural	3.1E-15	0.0E+00	8.7E-22	1.2E-12
Piperonyl butoxide	Soil	agricultural	7.5E-12	3.1E-19	1.2E-19	1.2E-10
Pirimicarb	Soil	agricultural	1.7E-10	0.0E+00	3.0E-17	6.8E-09
Polychlorinated biphenyls	Air		5.7E-11	4.5E-15	0.0E+00	1.0E-08
Polychlorinated biphenyls	Air	high. pop.	2.5E-14	2.0E-18	0.0E+00	4.6E-12
Polychlorinated biphenyls	Water		3.1E-14	4.5E-17	0.0E+00	2.3E-10
Prochloraz	Soil	agricultural	4.3E-06	4.4E-12	8.2E-12	4.2E-03
Procymidone	Soil	agricultural	3.4E-10	0.0E+00	9.8E-17	6.0E-09
Profenofos	Soil	agricultural	5.6E-11	0.0E+00	1.6E-16	1.6E-06
Prometryn	Soil	agricultural	3.0E-11	0.0E+00	1.0E-17	2.6E-07
Pronamide	Soil	agricultural	3.7E-06	5.8E-12	2.4E-12	9.7E-04
Propachlor	Soil	agricultural	1.7E-09	0.0E+00	5.9E-17	6.1E-07
Propanal	Air		3.9E-15	0.0E+00	0.0E+00	1.6E-15
Propanal	Air	high. pop.	6.1E-11	0.0E+00	0.0E+00	2.4E-11
Propanal	Air	low. pop.	1.4E-10	0.0E+00	0.0E+00	6.0E-11
Propanal	Water	river	3.0E-12	0.0E+00	0.0E+00	1.4E-10
Propargite	Soil	agricultural	1.5E-11	0.0E+00	4.0E-18	6.4E-10
Propene	Air		1.3E-10	0.0E+00	0.0E+00	0.0E+00
Propene	Air	high. pop.	1.4E-07	0.0E+00	0.0E+00	0.0E+00
Propene	Air	low. pop.	1.1E-08	0.0E+00	0.0E+00	0.0E+00
Propene	Water	river	8.2E-08	0.0E+00	0.0E+00	0.0E+00
Propiconazole	Air	low. pop.	7.9E-13	0.0E+00	1.0E-18	3.1E-10
Propiconazole	Water	groundwater	5.4E-16	0.0E+00	8.3E-21	2.7E-13
Propiconazole	Water	river	5.2E-20	0.0E+00	8.0E-25	1.2E-15
Propiconazole	Soil	agricultural	1.9E-11	0.0E+00	3.9E-17	9.5E-09
Propionic acid	Air		1.3E-12	0.0E+00	0.0E+00	8.9E-12
Propionic acid	Air	high. pop.	8.4E-09	0.0E+00	0.0E+00	6.0E-08
Propionic acid	Air	low. pop.	5.1E-09	0.0E+00	0.0E+00	3.3E-08
Propionic acid	Water	river	1.8E-08	0.0E+00	0.0E+00	1.3E-06
Propylamine	Air	high. pop.	7.3E-13	0.0E+00	0.0E+00	5.0E-13
Propylamine	Water	river	1.8E-12	0.0E+00	0.0E+00	4.7E-11
Propylene oxide	Air	high. pop.	3.9E-09	1.4E-15	2.6E-14	3.5E-09

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Propylene oxide	Water	river	9.0E-09	2.1E-15	2.2E-14	1.4E-07
Prosulfuron	Soil	agricultural	7.9E-13	0.0E+00	0.0E+00	5.2E-09
Pymetrozine	Soil	agricultural	1.5E-12	0.0E+00	0.0E+00	3.2E-10
Pyrene	Air		3.9E-14	1.3E-19	1.1E-20	2.0E-10
Pyrethrin	Soil	agricultural	8.1E-12	0.0E+00	0.0E+00	2.0E-07
Pyrimethanil	Soil	agricultural	1.1E-10	0.0E+00	0.0E+00	5.1E-09
Pyriithiobac sodium salt	Soil	agricultural	2.0E-12	0.0E+00	0.0E+00	2.8E-09
Quizalofop ethyl ester	Air	low. pop.	2.5E-13	0.0E+00	3.9E-19	3.3E-10
Quizalofop ethyl ester	Soil	agricultural	4.3E-11	0.0E+00	1.7E-16	2.2E-08
Rimsulfuron	Soil	agricultural	2.8E-12	0.0E+00	0.0E+00	1.8E-09
Rotenone	Soil	agricultural	4.6E-12	0.0E+00	2.0E-18	5.3E-10
Sethoxydim	Air	low. pop.	5.4E-13	0.0E+00	4.3E-20	2.2E-11
Sethoxydim	Soil	agricultural	2.2E-10	0.0E+00	6.7E-18	1.8E-09
Simazine	Soil	agricultural	4.2E-11	0.0E+00	6.9E-16	4.4E-07
Sodium formate	Air	high. pop.	2.2E-11	0.0E+00	0.0E+00	1.0E-11
Sodium formate	Water	river	5.3E-11	0.0E+00	0.0E+00	1.2E-10
Styrene	Air		1.2E-09	6.0E-16	1.2E-16	1.6E-11
Styrene	Air	high. pop.	2.6E-10	2.7E-16	5.3E-17	4.0E-12
Styrene	Air	low. pop.	2.1E-10	3.4E-18	6.7E-19	2.7E-12
Sulfentrazone	Air	low. pop.	5.1E-12	0.0E+00	0.0E+00	2.6E-08
Sulfentrazone	Soil	agricultural	2.9E-11	0.0E+00	0.0E+00	3.1E-07
Sulfosulfuron	Soil	agricultural	3.7E-14	0.0E+00	0.0E+00	4.4E-11
Sulfuric acid	Air		1.3E-10	0.0E+00	0.0E+00	6.2E-09
Sulfuric acid	Air	high. pop.	5.2E-11	0.0E+00	0.0E+00	2.6E-09
Sulfuric acid	Air	low. pop.	7.5E-09	0.0E+00	0.0E+00	3.5E-07
Sulfuric acid	Soil	agricultural	5.4E-09	0.0E+00	0.0E+00	3.0E-07
t-Butyl methyl ether	Air	high. pop.	4.9E-10	5.2E-17	8.7E-18	1.2E-11
t-Butyl methyl ether	Water	ocean	3.4E-11	9.3E-20	1.6E-20	1.7E-13
t-Butyl methyl ether	Water	river	2.0E-11	2.7E-19	8.7E-20	5.6E-11
t-Butylamine	Air	high. pop.	2.8E-12	0.0E+00	0.0E+00	2.6E-11
t-Butylamine	Water	river	6.6E-12	0.0E+00	0.0E+00	1.7E-09
Tebupirimphos	Soil	agricultural	1.8E-11	0.0E+00	0.0E+00	4.1E-07
Teflubenzuron	Soil	agricultural	1.3E-12	0.0E+00	6.1E-18	1.2E-09
Tefluthrin	Air	low. pop.	1.5E-14	0.0E+00	0.0E+00	4.3E-11
Tefluthrin	Water	groundwater	7.3E-20	0.0E+00	0.0E+00	3.2E-17
Tefluthrin	Water	river	1.0E-22	0.0E+00	0.0E+00	5.2E-16

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Tefluthrin	Soil	agricultural	1.4E-11	0.0E+00	0.0E+00	6.2E-09
Terbacil	Soil	agricultural	6.0E-10	0.0E+00	2.5E-15	1.9E-06
Terbufos	Soil	agricultural	5.3E-11	0.0E+00	1.8E-14	3.3E-07
Thiazole, 2-(thiocyanatemethylthio)benzo-	Soil	agricultural	4.5E-10	0.0E+00	0.0E+00	2.2E-07
Thidiazuron	Soil	agricultural	3.5E-12	0.0E+00	0.0E+00	3.3E-09
Thifensulfuron-methyl	Soil	agricultural	4.0E-14	0.0E+00	5.9E-20	2.1E-10
Thiodicarb	Air	low. pop.	2.6E-13	0.0E+00	7.5E-20	3.2E-10
Thiodicarb	Soil	agricultural	1.1E-14	0.0E+00	1.5E-21	1.3E-11
Thiram	Soil	agricultural	2.8E-06	0.0E+00	2.2E-13	9.1E-03
Toluene	Air		3.5E-07	1.6E-18	1.8E-14	4.4E-09
Toluene	Air	high. pop.	1.5E-07	6.9E-19	1.4E-14	1.9E-09
Toluene	Air	low. pop.	1.2E-07	5.4E-19	9.5E-16	1.4E-09
Toluene	Water		1.3E-08	1.7E-17	1.5E-16	2.9E-07
Toluene	Water	ocean	1.2E-08	2.4E-19	2.3E-17	3.4E-11
Toluene	Water	river	8.9E-08	1.2E-16	1.0E-15	2.0E-06
Toluene, 2-chloro-	Air	high. pop.	2.9E-11	0.0E+00	1.1E-17	4.6E-12
Toluene, 2-chloro-	Water	river	6.4E-11	0.0E+00	8.5E-18	4.7E-09
Triadimenol	Soil	agricultural	3.0E-13	0.0E+00	2.2E-19	5.5E-11
Triallate	Soil	agricultural	8.4E-14	0.0E+00	3.6E-19	5.7E-12
Triasulfuron	Soil	agricultural	2.5E-14	0.0E+00	1.9E-19	2.9E-11
Tribenuron-methyl	Soil	agricultural	8.8E-13	0.0E+00	1.1E-18	2.0E-11
Tribufos	Soil	agricultural	3.3E-11	0.0E+00	1.9E-15	2.3E-09
Trichlorfon	Soil	agricultural	2.3E-14	0.0E+00	4.0E-20	2.8E-10
Triclopyr	Soil	agricultural	9.1E-11	0.0E+00	0.0E+00	4.0E-08
Triethylene glycol	Water		3.8E-11	0.0E+00	0.0E+00	1.5E-11
Triethylene glycol	Water	ocean	1.2E-09	0.0E+00	0.0E+00	2.5E-17
Triethylene glycol	Water	river	3.8E-11	0.0E+00	0.0E+00	1.5E-11
Trifluralin	Air	low. pop.	7.4E-11	7.8E-18	7.7E-17	1.5E-08
Trifluralin	Soil	agricultural	1.7E-08	5.7E-15	5.6E-14	2.6E-06
Triforine	Soil	agricultural	1.4E-11	0.0E+00	3.7E-18	1.9E-09
Trimethylamine	Air	high. pop.	7.6E-13	0.0E+00	0.0E+00	1.1E-12
Trimethylamine	Water	river	1.8E-12	0.0E+00	0.0E+00	1.2E-10
Trinexapac-ethyl	Soil	agricultural	3.2E-11	0.0E+00	0.0E+00	1.6E-09
Urea	Water	river	3.6E-12	0.0E+00	0.0E+00	3.7E-11
Vinclozolin	Soil	agricultural	1.1E-10	0.0E+00	1.2E-16	2.2E-08

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Xylene	Air		2.1E-07	9.9E-16	2.3E-14	2.3E-09
Xylene	Air	high. pop.	9.3E-08	8.4E-16	2.0E-14	1.0E-09
Xylene	Air	low. pop.	5.6E-07	2.5E-16	5.7E-15	6.0E-09
Xylene	Water		6.4E-09	1.2E-17	7.7E-17	2.0E-07
Xylene	Water	ocean	7.3E-09	9.3E-19	1.7E-17	1.7E-11
Xylene	Water	river	5.4E-08	9.8E-17	6.5E-16	1.7E-06
Antimony	Soil	agricultural	9.5E-14	0.0E+00	4.5E-17	9.1E-09
Antimony	Soil		5.2E-12	0.0E+00	2.2E-15	5.0E-07
Antimony	Water	river	2.3E-08	0.0E+00	2.0E-11	4.4E-03
Antimony	Water	groundwater, long-term	1.4E-07	0.0E+00	1.1E-10	1.3E-02
Antimony	Water	groundwater	1.7E-09	0.0E+00	1.5E-12	1.7E-04
Antimony	Water		9.0E-11	0.0E+00	7.6E-14	1.7E-05
Antimony	Air	low. pop., long-term	2.3E-11	0.0E+00	1.4E-14	1.6E-06
Antimony	Air	low. pop.	4.7E-09	0.0E+00	2.8E-12	3.1E-04
Antimony	Air	high. pop.	2.3E-10	0.0E+00	1.4E-13	1.6E-05
Antimony	Air		4.5E-08	0.0E+00	2.8E-11	3.0E-03
Arsenic	Soil	industrial	1.5E-10	1.7E-13	1.3E-11	3.2E-06
Arsenic	Soil	agricultural	6.3E-10	9.6E-13	7.1E-11	1.3E-05
Arsenic	Soil		1.3E-11	1.5E-14	1.1E-12	2.7E-07
Arsenic	Water	river	2.3E-08	5.0E-11	3.7E-09	9.3E-04
Arsenic	Water	ocean	1.8E-09	6.0E-12	4.4E-10	2.5E-22
Arsenic	Water	groundwater, long-term	4.4E-07	9.6E-10	7.1E-08	9.4E-03
Arsenic	Water	groundwater	1.0E-08	2.2E-11	1.6E-09	2.2E-04
Arsenic	Water		2.2E-09	4.9E-12	3.6E-10	9.1E-05
Arsenic	Air	low. pop., long-term	1.4E-09	2.7E-12	2.0E-10	2.0E-05
Arsenic	Air	low. pop.	3.8E-08	7.6E-11	5.6E-09	5.7E-04
Arsenic	Air	high. pop.	3.9E-09	8.3E-12	5.6E-10	5.8E-05
Arsenic	Air		6.4E-11	1.3E-13	9.2E-12	9.5E-07
Barium	Soil	industrial	1.9E-07	0.0E+00	2.5E-10	3.0E-03
Barium	Soil	agricultural	9.3E-12	0.0E+00	1.2E-14	1.5E-07
Barium	Soil		3.3E-10	0.0E+00	4.3E-13	5.2E-06
Barium	Water	river	5.0E-07	0.0E+00	1.3E-09	1.6E-02
Barium	Water	ocean	2.9E-08	0.0E+00	7.5E-11	2.9E-20
Barium	Water	groundwater, long-term	2.0E-06	0.0E+00	5.1E-09	3.1E-02

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Barium	Water	groundwater	3.1E-09	0.0E+00	8.1E-12	4.9E-05
Barium	Water		2.3E-06	0.0E+00	6.0E-09	7.2E-02
Barium	Air	low. pop., long-term	1.5E-09	0.0E+00	2.6E-12	1.7E-05
Barium	Air	low. pop.	4.3E-08	0.0E+00	7.5E-11	4.8E-04
Barium	Air	high. pop.	1.1E-08	0.0E+00	1.9E-11	1.2E-04
Barium	Air		1.8E-08	0.0E+00	3.0E-11	2.0E-04
Beryllium	Water	river	7.8E-12	3.9E-37	2.1E-18	1.1E-07
Beryllium	Water	groundwater, long-term	1.2E-07	6.2E-33	3.3E-14	9.4E-04
Beryllium	Water	groundwater	3.3E-10	1.6E-35	8.8E-17	2.5E-06
Beryllium	Water		8.0E-11	4.0E-36	2.1E-17	1.1E-06
Beryllium	Air	low. pop., long-term	3.3E-11	3.1E-16	2.3E-13	1.7E-07
Beryllium	Air	low. pop.	1.5E-10	1.4E-15	1.0E-12	7.7E-07
Beryllium	Air	high. pop.	1.2E-10	1.3E-14	9.8E-12	6.1E-07
Beryllium	Air		4.1E-12	2.5E-16	1.9E-13	2.1E-08
Cadmium	Soil	industrial	3.8E-12	1.7E-16	4.5E-14	4.5E-06
Cadmium	Soil	agricultural	5.3E-08	4.9E-11	1.3E-08	6.2E-02
Cadmium	Soil		1.2E-11	5.4E-16	1.5E-13	1.4E-05
Cadmium	Water	river	5.3E-09	4.6E-13	1.2E-10	1.2E-02
Cadmium	Water	ocean	6.9E-10	6.6E-14	1.8E-11	4.4E-21
Cadmium	Water	groundwater, long-term	1.7E-07	1.5E-11	3.9E-09	2.0E-01
Cadmium	Water	groundwater	5.0E-10	4.4E-14	1.2E-11	5.9E-04
Cadmium	Water		9.4E-10	8.1E-14	2.2E-11	2.2E-03
Cadmium	Air	stratosphere + troposphere	1.7E-16	5.6E-20	1.5E-17	1.4E-10
Cadmium	Air	low. pop., long-term	3.5E-11	1.2E-14	3.1E-12	2.9E-05
Cadmium	Air	low. pop.	1.1E-08	3.6E-12	9.5E-10	8.9E-03
Cadmium	Air	high. pop.	2.7E-09	1.1E-12	2.3E-10	2.2E-03
Cadmium	Air		1.7E-10	6.4E-14	1.5E-11	1.4E-04
Chromium VI	Soil		6.7E-08	3.5E-09	7.8E-12	3.5E-03
Chromium VI	Water	river	1.3E-07	1.4E-08	3.1E-11	1.4E-02
Chromium VI	Water	groundwater, long-term	9.5E-07	9.7E-08	2.2E-10	5.0E-02
Chromium VI	Water	groundwater	4.1E-09	4.2E-10	9.5E-13	2.2E-04
Chromium VI	Water		5.1E-10	5.3E-11	1.2E-13	5.4E-05
Chromium VI	Air	low. pop., long-term	1.7E-10	1.4E-11	4.1E-14	6.2E-06

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Chromium VI	Air	low. pop.	8.5E-09	7.0E-10	2.1E-12	3.1E-04
Chromium VI	Air	high. pop.	1.7E-10	1.4E-11	1.6E-13	6.3E-06
Chromium VI	Air		2.6E-12	2.1E-13	1.5E-15	9.7E-08
Copper	Soil	industrial	5.7E-10	0.0E+00	4.2E-17	3.0E-03
Copper	Soil	agricultural		0.0E+00	1.0E-09	4.8E+01
Copper	Soil		4.2E-08	0.0E+00	3.2E-15	2.2E-01
Copper	Water	river	3.2E-08	0.0E+00	4.6E-15	3.2E-01
Copper	Water	ocean	1.2E-09	0.0E+00	7.6E-17	5.0E-23
Copper	Water	groundwater, long-term	2.4E-05	0.0E+00	3.4E-12	1.3E+02
Copper	Water	groundwater	3.8E-09	0.0E+00	5.4E-16	2.0E-02
Copper	Water		8.1E-09	0.0E+00	1.2E-15	8.1E-02
Copper	Air	stratosphere + troposphere	2.9E-14	0.0E+00	9.8E-19	1.1E-07
Copper	Air	low. pop., long-term	2.2E-09	0.0E+00	7.5E-14	8.0E-03
Copper	Air	low. pop.	1.1E-07	0.0E+00	3.8E-12	4.1E-01
Copper	Air	high. pop.	1.1E-08	0.0E+00	3.6E-13	3.9E-02
Copper	Air		2.5E-08	0.0E+00	8.5E-13	9.2E-02
Lead	Soil	industrial	1.7E-10	1.5E-17	5.3E-15	7.0E-08
Lead	Soil	agricultural	5.9E-07	9.0E-11	3.2E-08	2.4E-04
Lead	Soil		4.6E-10	4.0E-17	1.4E-14	1.9E-07
Lead	Water	river	3.0E-08	4.4E-15	1.6E-12	2.1E-05
Lead	Water	ocean	1.9E-09	1.5E-16	5.2E-14	1.3E-27
Lead	Water	groundwater, long-term	2.8E-07	4.1E-14	1.4E-11	1.1E-04
Lead	Water	groundwater	7.6E-10	1.1E-16	3.9E-14	3.1E-07
Lead	Water		8.1E-09	1.2E-15	4.2E-13	5.6E-06
Lead	Air	stratosphere + troposphere	3.4E-16	1.6E-20	5.5E-18	9.6E-14
Lead	Air	low. pop., long-term	2.3E-09	1.1E-13	3.7E-11	6.5E-07
Lead	Air	low. pop.	1.2E-07	5.5E-12	2.0E-09	3.4E-05
Lead	Air	high. pop.	1.7E-08	7.7E-13	2.7E-10	4.9E-06
Lead	Air		2.5E-08	1.1E-12	4.0E-10	7.0E-06
Mercury	Soil	industrial	7.6E-13	1.1E-16	1.2E-14	1.2E-08
Mercury	Soil	agricultural	4.2E-11	1.5E-12	1.8E-10	6.6E-07
Mercury	Water	river	4.6E-09	8.9E-13	1.1E-10	1.0E-04
Mercury	Water	ocean	1.1E-11	4.8E-15	5.7E-13	1.0E-26

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Mercury	Water	groundwater, long-term	1.9E-08	3.7E-12	4.4E-10	3.0E-04
Mercury	Water	groundwater	4.6E-11	8.9E-15	1.1E-12	7.1E-07
Mercury	Water		9.2E-11	1.8E-14	2.1E-12	2.0E-06
Mercury	Air	stratosphere + troposphere	1.2E-18	1.3E-20	1.6E-18	1.3E-14
Mercury	Air	low. pop., long-term	1.8E-11	2.0E-13	2.3E-11	1.9E-07
Mercury	Air	low. pop.	3.4E-09	3.8E-11	4.5E-09	3.7E-05
Mercury	Air	high. pop.	4.2E-10	4.4E-12	5.2E-10	4.4E-06
Mercury	Air		2.8E-09	3.0E-11	3.5E-09	2.9E-05
Molybdenum	Soil	agricultural	3.3E-11	0.0E+00	2.9E-13	4.9E-09
Molybdenum	Soil		7.3E-12	0.0E+00	5.0E-16	1.1E-09
Molybdenum	Water	river	6.5E-09	0.0E+00	8.7E-13	1.9E-06
Molybdenum	Water	ocean	5.1E-11	0.0E+00	5.7E-15	1.3E-26
Molybdenum	Water	groundwater, long-term	4.1E-07	0.0E+00	5.5E-11	6.1E-05
Molybdenum	Water	groundwater	1.5E-08	0.0E+00	2.1E-12	2.3E-06
Molybdenum	Water		1.8E-10	0.0E+00	2.5E-14	5.4E-08
Molybdenum	Air	low. pop., long-term	4.5E-10	0.0E+00	1.2E-12	4.7E-08
Molybdenum	Air	low. pop.	1.1E-09	0.0E+00	2.8E-12	1.1E-07
Molybdenum	Air	high. pop.	2.1E-09	0.0E+00	5.4E-12	2.2E-07
Molybdenum	Air		4.5E-09	0.0E+00	1.2E-11	4.7E-07
Nickel	Soil	industrial	5.7E-11	1.5E-14	8.2E-16	8.9E-06
Nickel	Soil	agricultural	8.7E-10	4.2E-13	2.3E-14	1.3E-04
Nickel	Soil		7.8E-11	2.0E-14	1.1E-15	1.2E-05
Nickel	Water	river	2.6E-08	1.3E-11	7.2E-13	7.7E-03
Nickel	Water	ocean	1.4E-09	6.9E-13	3.9E-14	1.5E-21
Nickel	Water	groundwater, long-term	7.9E-06	3.9E-09	2.2E-10	1.2E+00
Nickel	Water	groundwater	1.9E-08	9.2E-12	5.2E-13	2.9E-03
Nickel	Water		9.2E-09	4.5E-12	2.5E-13	2.8E-03
Nickel	Air	stratosphere + troposphere	1.2E-15	4.8E-19	2.7E-20	1.3E-10
Nickel	Air	low. pop., long-term	4.8E-10	1.9E-13	1.1E-14	5.1E-05
Nickel	Air	low. pop.	8.3E-08	3.3E-11	1.9E-12	9.0E-03
Nickel	Air	high. pop.	6.8E-08	2.7E-11	1.5E-12	7.3E-03
Nickel	Air		1.5E-09	6.2E-13	3.5E-14	1.7E-04
Silver	Soil	agricultural	5.3E-19	0.0E+00	6.0E-20	5.4E-14

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-cancer (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Silver	Soil		2.6E-13	0.0E+00	7.2E-17	2.6E-08
Silver	Water	river	4.9E-10	0.0E+00	2.6E-13	9.6E-05
Silver	Water	ocean	2.0E-11	0.0E+00	1.2E-14	3.7E-25
Silver	Water	groundwater, long-term	9.4E-09	0.0E+00	5.0E-12	9.5E-04
Silver	Water	groundwater	2.0E-10	0.0E+00	1.0E-13	2.0E-05
Silver	Water		1.7E-08	0.0E+00	8.9E-12	3.2E-03
Silver	Air	low. pop., long-term	3.9E-11	0.0E+00	1.3E-12	2.7E-06
Silver	Air	low. pop.	6.9E-13	0.0E+00	2.4E-14	4.9E-08
Silver	Air	high. pop.	1.4E-10	0.0E+00	4.7E-12	1.0E-05
Silver	Air		2.1E-13	0.0E+00	7.0E-15	1.5E-08
Thallium	Water	river	2.6E-10	0.0E+00	1.4E-11	9.1E-06
Thallium	Water	groundwater, long-term	1.7E-08	0.0E+00	9.4E-10	3.0E-04
Thallium	Water	groundwater	2.9E-11	0.0E+00	1.6E-12	5.1E-07
Thallium	Water		1.9E-11	0.0E+00	1.1E-12	6.8E-07
Thallium	Air	low. pop.	2.1E-12	0.0E+00	8.3E-14	2.6E-08
Thallium	Air	high. pop.	1.4E-10	0.0E+00	5.4E-12	1.7E-06
Thallium	Air		1.6E-11	0.0E+00	6.3E-13	2.0E-07
Vanadium	Soil	agricultural	3.3E-10	0.0E+00	4.3E-13	1.9E-05
Vanadium	Soil		2.6E-12	0.0E+00	3.2E-15	1.5E-07
Vanadium	Water	river	5.0E-09	0.0E+00	1.2E-11	5.6E-04
Vanadium	Water	ocean	1.6E-10	0.0E+00	4.7E-13	1.7E-22
Vanadium	Water	groundwater, long-term	4.9E-07	0.0E+00	1.2E-09	2.9E-02
Vanadium	Water	groundwater	9.3E-10	0.0E+00	2.2E-12	5.4E-05
Vanadium	Water		2.2E-10	0.0E+00	5.2E-13	2.5E-05
Vanadium	Air	low. pop., long-term	1.6E-09	0.0E+00	3.0E-12	6.5E-05
Vanadium	Air	low. pop.	1.2E-08	0.0E+00	2.3E-11	5.1E-04
Vanadium	Air	high. pop.	2.4E-07	0.0E+00	4.3E-10	9.7E-03
Vanadium	Air		5.5E-10	0.0E+00	1.0E-12	2.3E-05
Zinc	Soil	industrial	6.0E-09	0.0E+00	3.4E-12	4.4E-04
Zinc	Soil	agricultural	1.1E-06	0.0E+00	2.2E-08	8.0E-02
Zinc	Soil		2.0E-08	0.0E+00	1.1E-11	1.4E-03
Zinc	Water	river	5.2E-07	0.0E+00	5.4E-10	7.0E-02
Zinc	Water	ocean	7.9E-08	0.0E+00	9.5E-11	1.8E-20
Zinc	Water	groundwater, long-term	1.4E-05	0.0E+00	1.4E-08	1.0E+00

Substance	Compart.	Sub-Compart.	Mass (kg)	Human non-can (cases)	Human cancer (cases)	Ecotoxicity (PAFm ³ day)
Zinc	Water	groundwater	5.0E-08	0.0E+00	5.1E-11	3.7E-03
Zinc	Water		1.8E-08	0.0E+00	1.9E-11	2.4E-03
Zinc	Air	stratosphere + troposphere	1.7E-14	0.0E+00	1.1E-16	8.6E-10
Zinc	Air	low. pop., long-term	1.7E-09	0.0E+00	1.1E-11	8.5E-05
Zinc	Air	low. pop.	1.9E-07	0.0E+00	1.2E-09	9.5E-03
Zinc	Air	high. pop.	2.7E-08	0.0E+00	1.7E-10	1.4E-03
Zinc	Air		5.1E-08	0.0E+00	3.3E-10	2.6E-03

SI IV.6 Parameters for dynamic LCA

Table SI IV.6. Parameters requested by the dynamic LCI model (from Tiruta-Barna et al., 2016)

	Parameter	Name	Significance
Process model (specific for process i)	$\alpha(t)$	Production function	Describes the time shape of the activity (e.g. continuous, constant, discontinuous...)
	$\beta(t)$	Environmental intervention function	Describe the time shape of the emissions/resource consumptions. Usually linked to $\alpha(t)$
	r	Production period	Time between the earliest input (raw material) and the latest output of the activity
	T	Representative period	Life time of the main infrastructure (material support) related to the activity
	t_0	Start date of the analysis	Arbitrary or calendar dependent
Supply model (process link i-j)	δ	Delay	Storage time, no activity takes place
	τ	Supply period	Supply frequency for intermittent supply; $\tau=T$ for continuous supply

Table SI IV.7– Temporal parameters for dynamic LCI calculation (related to the functional unit, 1 kg of grape).

Process	T (years)	r (days)	τ (days)	α (kg.day ⁻¹)	β (kg.day ⁻¹)
Grape production	25	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 4/12, 0,$ $\text{if}(x < 10/12, (12/5)/$ $25, 0))$	<u>Pesticides</u> $x := t - \text{trunc}(t) ;$ $b^1 * (1/10) * \text{if}(x < 4/12, 0, \text{if}(x < 11/1$ $2, \text{if}((x * 12 -$ $\text{trunc}(x * 12)) < 0.25, 6.855, 0), 0))$ $\left\{ \begin{array}{l} 0, \quad \text{month} < 4 \\ b^1 * 0.6855, \quad 4 \leq \text{month} < 11 \\ \quad \quad \quad \text{and week} = 1 \\ 0, \quad \quad \quad \text{month} \geq 11 \end{array} \right.$ <u>N₂O</u> 1/25
Pesticides production	50	1	182.5	1/50	1/50
Fertilizers production	50	1	182.5	1/50	1/50
Irrigation	1	1	0	1	1
Electricity production	30	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 10/12, 0, 6)$	$x := t - \text{trunc}(t) ; \text{if}(x < 10/12, 0,$ $6)$ $\left\{ \begin{array}{l} 0, \quad \text{month} < 10 \\ 6, \quad \text{month} \geq 10 \end{array} \right.$
Fertilising, by broadcaster	1	365	365	$x := t - \text{trunc}(t) ;$ $\text{if}(x < 5/12, 0,$ $\text{if}(x < 5.25/12, 24, \text{if}$ $(x < 8/12, 0, \text{if}(x < 8.$ $25, 24, 0))))$	$x := t - \text{trunc}(t) ; \text{if}(x < 5/12, 0,$ $\text{if}(x < 5.25/12, 24, \text{if}(x < 8/12, 0, \text{if}(x$ $< 8.25, 24, 0))))$ $\left\{ \begin{array}{l} 0, \quad \text{month} < 5 \\ 24, \quad 5 \leq \text{month} < 5.25 \\ 0, \quad 5.25 \leq \text{month} < 8 \\ 24, \quad 8 \leq \text{month} < 8.25 \\ 0, \quad \text{month} \geq 8.25 \end{array} \right.$

¹ b represents the values of pesticides emissions for the “grape production” dataset, obtained from the matrix of environmental interventions (SimaPro/ecoinvent)

Table SI IV.8 – Supply parameters for the dynamic LCI model (related to the functional unit, 1 kg of grape).

Producer	Consumer	Continuous	Supply model	
Pesticides	Grape production	No	$a = \text{see } ^2$	$\delta = 60$ days
Fertilizers	Grape production	No	$a = \text{see } ^2$	$\delta = 60$ days
Irrigation	Grape production	No	$a = -0.177$	$\delta = 0$ days
Electricity	Grape production	No	$a = -0.090$	$\delta = 0$ days
Fertilising, by broadcaster	Grape production	No	$a = 7.33 \times 10^{-4}$	$\delta = 0$ days

² represents the demand of pesticides or fertilizers by the foreground process (from technological matrix extracted from SimaPro/ecoinvent for the testbed case). Values can be found in the dataset presented in SI IV.4.

SI IV.7 Dynamic and conventional toxicity results

Toxicity results of Prochloraz and Copper for the testbed case of production of 1 kg of grape

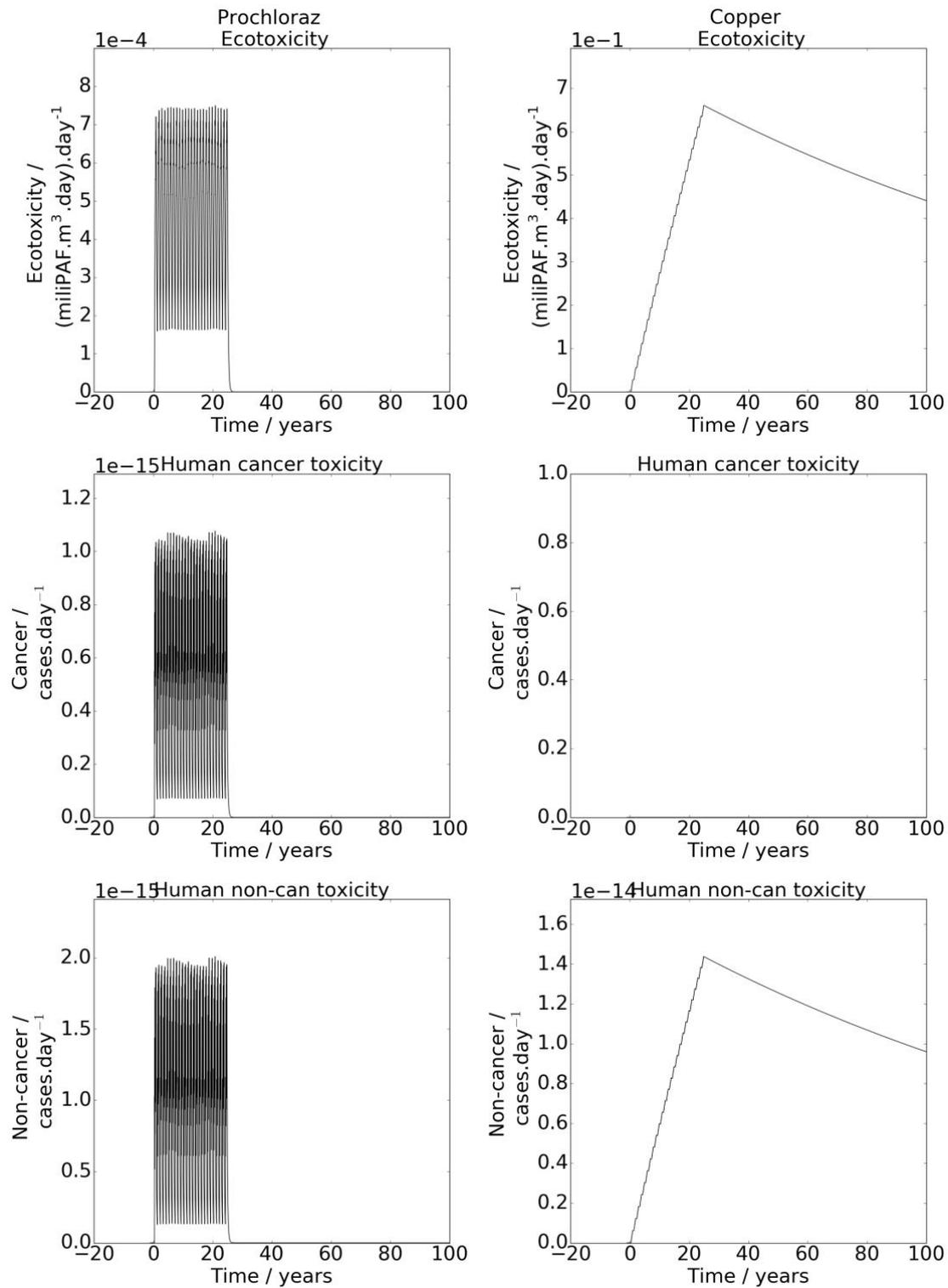


Figure SI IV.1 – Current Ecotoxicity $n_{eco}(t)$ (A), cancer (B) and non-cancer (C) human toxicity $n_{human}(t)$ of Prochloraz for the production of 1 kg of grapes

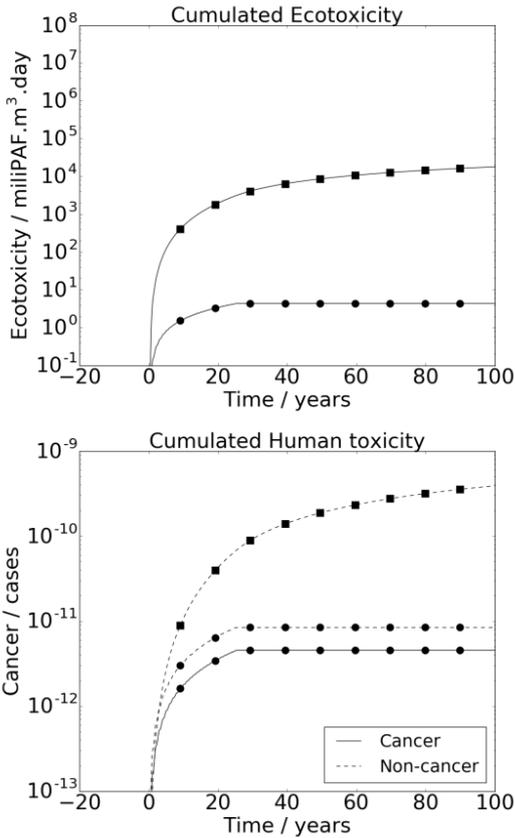


Figure SI IV.2 – Cumulated dynamic ecotoxicity $n_{eco,cumul}$ (A) and human toxicity $n_{human,cumul}$ (B) of prochloraz (●) and copper (■) for the production of 1 kg of grapes.

SI IV.8 Contribution of individual pesticides to total toxicity impacts

Table SI IV.9 – Contribution of organic pesticides on dynamic and conventional toxicity impacts. Results for human toxicity (Cancer and Non-cancer) and ecotoxicity (Eco) impacts for the production of 1 kg of grape. The values for dynamic approach represent cumulated (eco)toxicity at 100 years.

Substance	Dynamic (100 years)			Conventional		
	Cancer	Non-cancer	Eco	Cancer	Non-cancer	Eco
Folpet	0.0%	0.0%	0.2%	0.0%	0.0%	0.0%
Thiram	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Imidacloprid	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Napropamide	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Chlorothalonil	0.0%	0.0%	0.3%	0.0%	0.0%	0.1%
Pronamide	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Pendimethalin	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Metolachlor	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Prochloraz	0.1%	0.0%	0.0%	0.0%	0.0%	0.0%
Mancozeb	0.0%	0.0%	0.3%	0.0%	0.0%	0.1%
Metiram	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
MCPB	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Glyphosate	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Chlormequat	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
2,4-D	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Metam-sodium dihydrate	0.0%	0.0%	0.7%	0.0%	0.0%	0.1%
Chlortoluron	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Isoproturon	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Metamitron	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Metazachlor	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Aclonifen	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%
Dimethenamid	0.0%	0.0%	0.1%	0.0%	0.0%	0.0%

SI V Sensitivity analysis of temporal parameters in a dynamic LCA framework

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SI V.1 Dynamic effluent for the WWTP case study

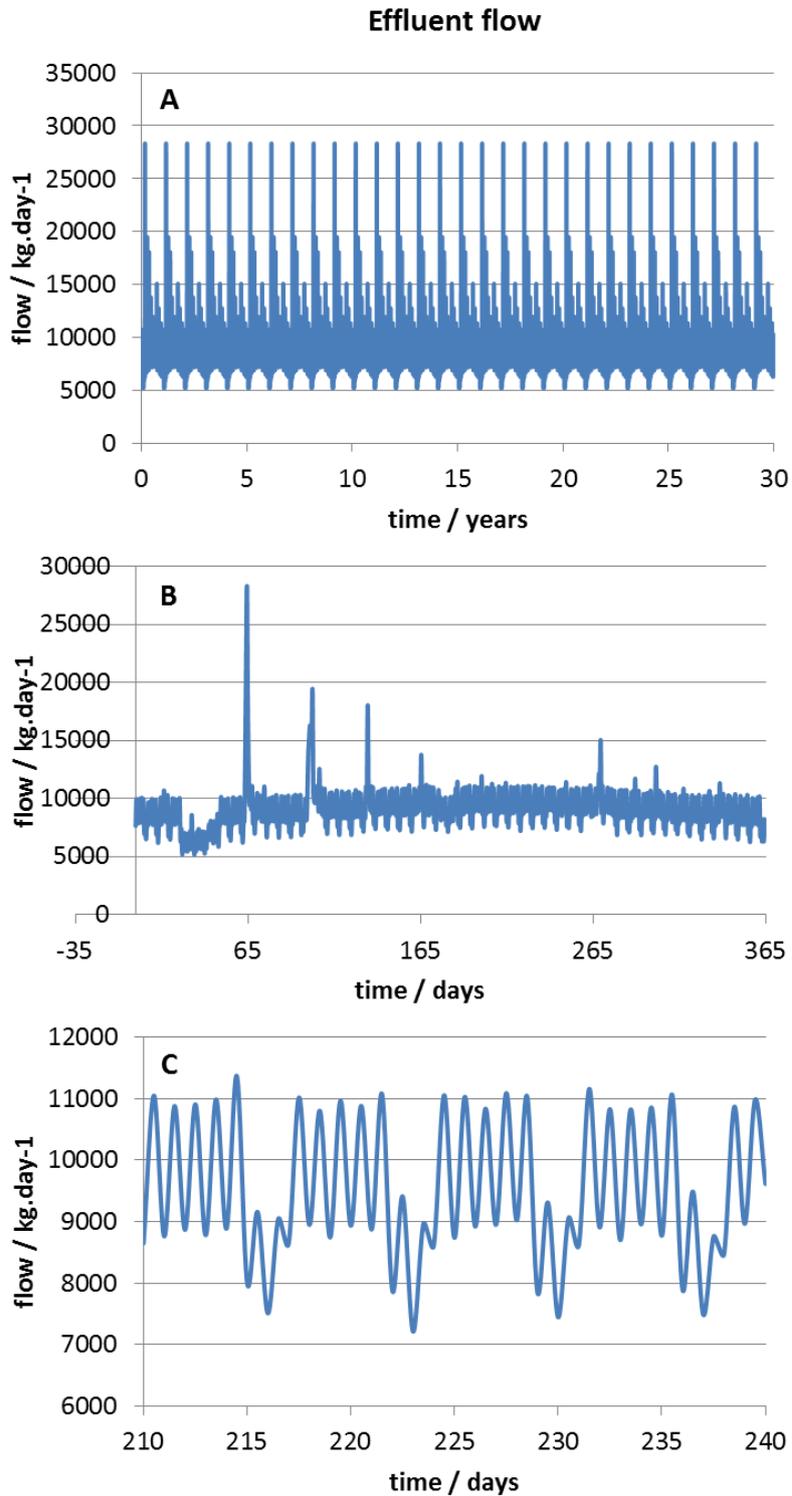


Figure SI V.1 – Dynamic effluent flow for the case study of a WWTP. Three different time periods for the effluent flow are shown: A represents the representative period of 30 years; B represents a period of 1 year (first year); and C represents a period of 1 month (month 7).

SI V.2 Conventional and dynamic data for WWTP case study inventory.

Table SI V.1 – Conventional inventory for the case study of a WWTP.

Process	Operational data	Ecoinvent process	Unit	Value	
WWTP	Infrastructure	wastewater treatment plant, class 2, CH	unit	2.3E-09	
	Electricity	electricity mix [FR]	kWh	4.0E-01	
	Methanol	methanol, at plant, GLO	kg	1.7E-02	
	Iron chloride	iron (III) chloride, 40% in H ₂ O, at plant, CH	kg	6.2E-02	
	Incineration		kg	3.2E-02	
	Emission		carbon dioxide, fossil [air/ high population]	kg	7.6E-04
			methane, fossil [air/ high population]	kg	7.4E-17
			dinitrogen monoxide [air/ high population]	kg	6.1E-07
			copper [water/ unspecified]	kg	3.4E-08
			lead [water/ unspecified]	kg	1.1E-08
			zinc [water/ unspecified]	kg	1.2E-07
		Methane, dichloro-, HCC-30 [water/ unspecified]	kg	6.8E-08	

Table SI V.2 – Process relative dynamic parameters for the case study of a WWTP (T and r in year; α and β present a unit which is the ones presented in table SI V.1 by year).

Process	Process model					
WWTP	$\alpha = \text{see}^1$	$\beta = \text{see}^1$			T=30	r=see ¹
Electricity	$\alpha = 0.02$	$\beta_{\text{CO}_2} = 9.4\text{E-}7$	$B_{\text{N}_2\text{O}} = 1.4\text{E-}9$	$\beta_{\text{CH}_4} = 2.1\text{E-}11$	T=50	r=0.0027367
Methanol	$\alpha = 0.033$	$\beta_{\text{CO}_2} = 5.1\text{E-}7$	$\beta_{\text{N}_2\text{O}} = 3.4\text{E-}9$	$\beta_{\text{CH}_4} = 3.8\text{E-}12$	T=30	r=0.0027367
Iron chloride	$\alpha = 0.02$	$\beta_{\text{CO}_2} = 1.3\text{E-}6$	$\beta_{\text{N}_2\text{O}} = 2.3\text{E-}9$	$B_{\text{CH}_4} = 4.0\text{E-}11$	T=50	r=0.0027367
Infrastructure	$\alpha = 0.333$	$\beta_{\text{CO}_2} = 1.8\text{E-}3$		$B_{\text{CH}_4} = 2.8\text{E-}6$	T=3	r=3
		$B_{\text{N}_2\text{O}} = 1.8\text{E-}8$		$B_{\text{Pb}} = 2.9\text{E-}10$		
Incineration	$\alpha = 0.02$	$\beta_{\text{CO}_2} = 2.1\text{E-}7$		$\beta_{\text{Cu}} = 4.1\text{E-}10$	T=50	r=0.0027367
		$\beta_{\text{Zn}} = 2.3\text{E-}9$		$\beta_{\text{Pb}} = 3.9\text{E-}10$		

¹ Temporal characteristics of this process was simulated in other software called Sumo.

Table SI V.3 – Supply chain relative dynamic parameters for the case study of a WWTP (δ in year and a presents the same units as in table SI V.1).

Producer	Consumer	Supply model	
Electricity	WWTP	cont ($a = -4.0E-01$)	$\delta = 0$
Methanol	WWTP	$a = -1.7E-02$	$\delta = 0.164$
Iron chloride	WWTP	$a = -6.2E-02$	$\delta = 0.164$
Infrastructure	WWTP	$a = -2.3E-09$	$\delta = 0.5$
Incineration	WWTP	$a = -3.2E-02$	$\delta = 0.019$

SI V.3 Dynamic impact results for the case study of WTTP.

The table below presents the time step size used for the calculations of dynamic LCI and dynamic LCIA, on a basis of 365.24 days/year.

Table SI V.4 – Time step size in common units used for the dynamic calculation and their correspondence in days

Time step size in common units	0.5 day	1 day	1 week	1 month	1 season	1 year
Time step size in days	0.5	1	7	30.44	91.31	365.24

Table below shows the relative difference between the cumulated values for the dynamic toxicity impact between the different step sizes and the reference interval of 1 year. The results for organic, inorganic and all substances show that the results for cumulated dynamic ecotoxicity and human toxicity do not have an important difference for different step sizes, at 100 years.

Table SI V.5 – Relative difference between cumulated values for toxicity impact for organic, inorganic and all substances. Results for different dynamic LCIA time step sizes (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year), for a calculation time span of 100 years

All substances			
	Ecotoxicity	Human cancer	Human non-cancer
0.5 day	1.6%	1.7%	1.7%
1 day	1.6%	1.7%	1.7%
1 week	1.5%	1.5%	1.6%
1 month	1.4%	1.7%	1.6%
1 season	1.0%	0.9%	1.0%
Organic substances			
	Ecotoxicity	Human cancer	Human non-cancer
0.5 day	0.8%	0.8%	0.8%
1 day	0.8%	0.8%	0.8%
1 week	0.8%	0.8%	0.8%
1 month	0.8%	0.8%	0.8%
1 season	0.5%	0.8%	0.8%
Inorganic substances			
	Ecotoxicity	Human cancer	Human non-cancer
0.5 day	1.6%	1.7%	1.7%
1 day	1.6%	1.7%	1.7%
1 week	1.5%	1.5%	1.6%
1 month	1.4%	1.5%	1.4%
1 season	1.0%	1.0%	1.1%

The influence of the integration time step for climate change impact calculation (convolution product calculation) is represented in table below.

Table SI V.6 - Dynamic mean temperature change - values calculated for 100 years. Results for different time steps (0.5 day, 1 day, 1 week, 1 month, 1 season and 1 year) for the dynamic model resolution. In all calculations, the inventory time step was fixed to 1 year.

ΔT value at year 100 (K)	0.5 day	1 day	1 week	1 month	1 season	1 year
Carbon dioxide	5.5E-17	5.5E-17	5.5E-17	5.5E-17	5.6E-17	5.8E-17
Methane	6.0E-19	6.0E-19	6.0E-19	6.0E-19	6.0E-19	6.3E-19
Dinitrogen monoxide	8.6E-20	8.6E-20	8.6E-20	8.6E-20	8.7E-20	9.1E-20
Total	5.6E-17	5.6E-17	5.6E-17	5.6E-17	5.6E-17	5.9E-17

SI VI Case study French mix

SI VI.1 Life cycle inventory for high and low nuclear energy use in the French electricity

mix

Table SI VI.1.1 – Life cycle inventory for high and low nuclear energy use in the French electricity mix

Process	Operational data	Process / Ecoinvent process	Unit	Value
French mix	Foreground process	French mix 2010 – 2030	MJ	0.382
	Foreground process	French mix 2030 – 2050	MJ	0.308
	Foreground process	French mix 2050 – 2070 (high nuclear scenario) *	MJ	0.31
	Foreground process	French mix 2050 – 2070 (low nuclear scenario)*	MJ	0.31
French mix 2010 – 2030	Electricity Coal	Electricity, high voltage {FR} electricity production, hard coal Alloc Def, U	MJ	0.033
	Electricity Oil	Electricity, high voltage {FR} electricity production, oil Alloc Def, U	MJ	0.011
	Electricity Natural gas	Electricity, high voltage {FR} electricity production, natural gas, combined cycle power plant Alloc Def, U	MJ	0.02
	Electricity	Electricity, for reuse in municipal waste incineration only {FR} treatment of municipal solid waste, incineration Alloc Def, U	MJ	0.002
	Electricity Geothermal	Electricity, high voltage {CH} electricity production, deep geothermal Alloc Def, U	MJ	0.001
	Electricity Sea	Electricity, high voltage {FR} electricity production, hydro, reservoir, alpine region Alloc Def, U	MJ	0.001
	Electricity Hydro	Electricity, high voltage {FR} electricity production, hydro, run-of-river Alloc Def, U	MJ	0.121
	Electricity Nuclear	Electricity, high voltage {FR} electricity production, nuclear, pressure water reactor Alloc Def, U	MJ	0.773
	Electricity Wind	Electricity, high voltage {FR} electricity production, wind, >3MW turbine, onshore Alloc Def, U	MJ	0.027
	Electricity Biogas	Electricity, high voltage {FR} heat and power co-generation, biogas, gas engine Alloc Def, U	MJ	0.002
	Electricity Wood	Electricity, high voltage {FR} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Def, U	MJ	0.002
Electricity Photovoltaic	Electricity, low voltage {FR} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Alloc Def, U	MJ	0.007	

Process	Operational data	Process / Ecoinvent process	Unit	Value
French mix 2030 – 2050	Electricity	Electricity, for reuse in municipal waste incineration only {FR} treatment of municipal solid waste, incineration Alloc Def, U	MJ	0.01
	Electricity	Electricity, high voltage {CH} electricity production, deep geothermal Alloc Def, U	MJ	0.003
	Electricity	Electricity, high voltage {FR} electricity production, hydro, reservoir, alpine region Alloc Def, U	MJ	0.013
	Electricity	Electricity, high voltage {FR} electricity production, hydro, run-of-river Alloc Def, U	MJ	0.112
	Electricity	Electricity, high voltage {FR} electricity production, nuclear, pressure water reactor Alloc Def, U	MJ	0.516
	Electricity	Electricity, high voltage {FR} electricity production, wind, >3MW turbine, onshore Alloc Def, U	MJ	0.238
	Electricity	Electricity, high voltage {FR} heat and power co-generation, biogas, gas engine Alloc Def, U	MJ	0.002
	Electricity	Electricity, high voltage {FR} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Def, U	MJ	0.01
	Electricity	Electricity, low voltage {FR} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Alloc Def, U	MJ	0.096
French mix 2050 – 2070 (high nuclear scenario)	Electricity	Electricity, for reuse in municipal waste incineration only {FR} treatment of municipal solid waste, incineration Alloc Def, U	MJ	0.006
	Electricity	Electricity, high voltage {CH} electricity production, deep geothermal Alloc Def, U	MJ	0.003
	Electricity	Electricity, high voltage {FR} electricity production, hydro, reservoir, alpine region Alloc Def, U	MJ	0.012
	Electricity	Electricity, high voltage {FR} electricity production, hydro, run-of-river Alloc Def, U	MJ	0.107
	Electricity	Electricity, high voltage {FR} electricity production, nuclear, pressure water reactor Alloc Def, U	MJ	0.495
	Electricity	Electricity, high voltage {FR} electricity production, wind, >3MW turbine, onshore Alloc Def, U	MJ	0.229
	Electricity	Electricity, high voltage {FR} heat and power co-generation, biogas, gas engine Alloc Def, U	MJ	0.051
	Electricity	Electricity, high voltage {FR} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Def, U	MJ	0.006
	Electricity	Electricity, low voltage {FR} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Alloc Def, U	MJ	0.092

Process	Operational data	Process / Ecoinvent process	Unit	Value
French mix 2050 – 2070 (low nuclear scenario)	Electricity	Electricity, for reuse in municipal waste incineration only {FR} treatment of municipal solid waste, incineration Alloc Def, U	MJ	0.006
	Electricity	Electricity, high voltage {CH} electricity production, deep geothermal Alloc Def, U	MJ	0.006
	Electricity	Electricity, high voltage {FR} electricity production, hydro, reservoir, alpine region Alloc Def, U	MJ	0.1
	Electricity	Electricity, high voltage {FR} electricity production, hydro, run-of-river Alloc Def, U	MJ	0.147
	Electricity	Electricity, high voltage {FR} electricity production, nuclear, pressure water reactor Alloc Def, U	MJ	0.191
	Electricity	Electricity, high voltage {FR} electricity production, wind, >3MW turbine, onshore Alloc Def, U	MJ	0.348
	Electricity	Electricity, high voltage {FR} heat and power co-generation, biogas, gas engine Alloc Def, U	MJ	0.052
	Electricity	Electricity, high voltage {FR} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Def, U	MJ	0.006
	Electricity	Electricity, low voltage {FR} electricity production, photovoltaic, 570kWp open ground installation, multi-Si Alloc Def, U	MJ	0.159

Some adaptations were done in order to develop the French electricity mix scenarios. No activity which considers sea as source was available in ecoinvent 3.2 database. Thus, this process was replaced by the activity “Electricity, high voltage {FR}| electricity production, hydro, reservoir, alpine region | Alloc Def, U” in order to account one activity in the mix scenarios. Also, French geography for the geothermal electricity activity and, for this reason, it was replaced by the Swiss geography (CH).

SI VI.2 Temporal parameters for the French electricity scenarios

Table SI VI.2.1– process-relative temporal parameters for the foreground processes for the French electricity mix scenarios.

Process	Process model			
French mix	$\alpha=1/20$	$\beta=1/20*b = 0$	T=20	r=0.00274
French mix 2010 – 2030	$\alpha=1/20$	$\beta=1/20*b = 0$	T=20	r=0.00274
French mix 2030 – 2050	$\alpha=1/20$	$\beta=1/20*b = 0$	T=20	r=0.00274
French mix 2050 – 2070 (high nuclear scenario)	$\alpha=1/20$	$\beta=1/20*b = 0$	T=20	r=0.002747
French mix 2050 – 2070 (low nuclear scenario)	$\alpha=1/20$	$\beta=1/20*b = 0$	T=20	r=0.00274

Value of b_{ij} parameter is zero because the “mix” activity has no direct emissions

The process French mix (functional unit process) has no emissions and it is not a real process. It was created in order to allow the proper creation of the three blocks of 20 years for the scenarios of 2010-2030, 2030-2050 and 2050-2070 (the latter present differences between the two scenarios studied). Each block is emplaced in different moments of time thanks to δ parameter.

Table SI VI.2.2 - supply-relative temporal parameters for the foreground processes for the French electricity mix scenarios

Producer	Consumer	Supply model		
French mix 2010 – 2030	French mix	cont (a = -3.8E-01)	$\delta = 40$	$\tau = T_c$
French mix 2030 – 2050	French mix	cont (a = -3.1E-01)	$\delta = 20$	$\tau = T_c$
French mix 2050 – 2070 (high nuclear scenario)	French mix	cont (a = -3.1E-01)	$\delta = 0$	$\tau = T_c$
French mix 2050 – 2070 (low nuclear scenario)	French mix	cont (a = -3.1E-01)	$\delta = 0$	$\tau = T_c$

SI VI.3 Contribution of substances in dynamic LCA (cut-off 1%).

Table SI VI.3.1 – Substances contribution for dynamic climate change calculated for 100 years

Substance	Air sub compartment	low nuclear electricity mix		high nuclear electricity mix	
		mean temperature change (contribution%) / K	radiative forcing (contribution%) / W.m-2yr	mean temperature change (contribution%) / K	radiative forcing (contribution%) / W.m-2yr
Methane, fossil	low. pop.	2.1E-19 (7.0%)	7.0E-17 (17.0%)	2.1E-19 (7.4%)	6.9E-17 (0.0%)
Methane, fossil	high. pop.	7.5E-21 (0.0%)	5.9E-18 (1.0%)	6.8E-21 (0.2%)	5.2E-18 (0.0%)
Carbon dioxide, fossil	high. pop.	6.2E-19 (21.0%)	8.1E-17 (19.0%)	5.9E-19 (20.4%)	7.6E-17 (0.0%)
Carbon dioxide, fossil	low. pop.	1.4E-18 (48.0%)	1.7E-16 (41.0%)	1.4E-18 (49.8%)	1.7E-16 (0.0%)
Carbon dioxide, fossil		3.9E-19 (13.0%)	5.1E-17 (12.0%)	3.4E-19 (11.8%)	4.3E-17 (0.0%)
Carbon dioxide, land transformation	low. pop.	6.1E-20 (2.0%)	8.4E-18 (2.0%)	6.1E-20 (2.1%)	8.4E-18 (0.0%)

Substance	Air sub compartment	low nuclear electricity mix		high nuclear electricity mix	
		mean temperature change (contribution%) / K	radiative forcing (contribution%) / W.m-2yr	mean temperature change (contribution%) / K	radiative forcing (contribution%) / W.m-2yr
Carbon dioxide, land transformation		2.3E-20 (1.0%)	3.1E-18 (1.0%)	2.3E-20 (0.8%)	3.1E-18 (0.0%)
Dinitrogen monoxide	high. pop.	3.7E-20 (1.0%)	5.3E-18 (1.0%)	3.7E-20 (1.3%)	5.2E-18 (0.0%)
Dinitrogen monoxide	low. pop.	4.9E-20 (2.0%)	7.1E-18 (2.0%)	4.9E-20 (1.7%)	7.1E-18 (0.0%)
Ethane, 1,2-dichloro-1,1,2,2-tetrafluoro-, CFC-114	low. pop.	8.5E-20 (3.0%)	8.4E-18 (2.0%)	1.0E-19 (3.5%)	1.1E-17 (0.0%)
Methane, biogenic	low. pop.	4.4E-21 (0.0%)	3.6E-18 (1.0%)	4.3E-21 (0.2%)	3.5E-18 (0.0%)

Table SI VI.3. – Substances contribution for dynamic toxicity calculated for 100 years

substance (compartment/subcompartment)	low nuclear electricity mix			high nuclear electricity mix		
	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.day	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.day
Arsenic (Air/high. pop.)	5.7E-14 (0.4%)	1.5E-12 (0.3%)	1.1E-06 (0.0%)	5.6E-14 (0.4%)	1.5E-12 (0.3%)	1.1E-06 (0.0%)
Arsenic (Air/low. pop., long-term)	8.5E-13 (6.0%)	5.2E-11 (9.9%)	4.3E-05 (0.0%)	1.1E-12 (7.5%)	6.6E-11 (13.4%)	5.4E-05 (0.0%)
Arsenic (Air/low. pop.)	9.3E-13 (6.6%)	5.9E-11 (11.2%)	4.8E-05 (0.0%)	7.4E-13 (5.2%)	4.7E-11 (9.5%)	3.8E-05 (0.0%)
Benzo(a)pyrene (Air/low. pop.)	2.2E-12 (15.4%)	0.0E+00 (0.0%)	5.1E-08 (0.0%)	1.8E-12 (12.8%)	0.0E+00 (0.0%)	4.3E-08 (0.0%)
Cadmium (Air/high. pop.)	1.5E-14 (0.1%)	2.8E-12 (0.5%)	3.4E-05 (0.0%)	1.5E-14 (0.1%)	2.8E-12 (0.6%)	3.3E-05 (0.0%)
Cadmium (Air/low. pop., long-term)	4.5E-14 (0.3%)	1.2E-11 (2.2%)	1.3E-04 (0.0%)	5.5E-14 (0.4%)	1.4E-11 (2.9%)	1.6E-04 (0.0%)
Cadmium (Air/low. pop.)	6.2E-13 (4.4%)	1.6E-10 (30.4%)	1.8E-03 (0.0%)	4.9E-13 (3.5%)	1.3E-10 (25.8%)	1.4E-03 (0.0%)
Chromium VI (Air/low. pop., long-term)	3.7E-12 (26.5%)	7.5E-14 (0.0%)	4.0E-05 (0.0%)	4.5E-12 (31.7%)	9.0E-14 (0.0%)	4.7E-05 (0.0%)
Chromium VI (Air/low. pop.)	2.7E-12 (19.0%)	5.3E-14 (0.0%)	2.8E-05 (0.0%)	2.7E-12 (19.0%)	5.3E-14 (0.0%)	2.8E-05 (0.0%)

substance (compartment/ subcompartment)	low nuclear electricity mix			high nuclear electricity mix		
	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.day	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.day
Dioxin, 2,3,7,8 Tetrachlorodibenzo-p- (Air/)	8.9E-14 (0.6%)	0.0E+00 (0.0%)	6.9E-10 (0.0%)	7.6E-14 (0.5%)	0.0E+00 (0.0%)	5.9E-10 (0.0%)
Formaldehyde (Air/high. pop.)	5.3E-13 (3.7%)	5.5E-15 (0.0%)	3.8E-07 (0.0%)	5.2E-13 (3.7%)	5.5E-15 (0.0%)	3.7E-07 (0.0%)
Lead (Air/low. pop., long-term)	7.1E-14 (0.5%)	2.5E-11 (4.8%)	6.3E-07 (0.0%)	9.1E-14 (0.6%)	3.2E-11 (6.5%)	7.8E-07 (0.0%)
Lead (Air/low. pop.)	1.4E-13 (1.0%)	5.1E-11 (9.6%)	1.2E-06 (0.0%)	1.2E-13 (0.8%)	4.0E-11 (8.2%)	9.5E-07 (0.0%)
Lead (Air/)	7.9E-15 (0.1%)	2.8E-12 (0.5%)	6.8E-08 (0.0%)	6.7E-15 (0.0%)	2.3E-12 (0.5%)	5.8E-08 (0.0%)
Mercury (Air/high. pop.)	2.4E-14 (0.2%)	2.8E-12 (0.5%)	4.8E-08 (0.0%)	2.2E-14 (0.2%)	2.6E-12 (0.5%)	4.5E-08 (0.0%)
Mercury (Air/low. pop., long-term)	6.2E-14 (0.4%)	7.4E-12 (1.4%)	1.1E-07 (0.0%)	7.9E-14 (0.6%)	9.4E-12 (1.9%)	1.3E-07 (0.0%)
Mercury (Air/low. pop.)	6.2E-14 (0.4%)	7.3E-12 (1.4%)	1.0E-07 (0.0%)	5.6E-14 (0.4%)	6.6E-12 (1.3%)	9.1E-08 (0.0%)
Mercury (Air/)	1.8E-13 (1.3%)	2.2E-11 (4.1%)	3.3E-07 (0.0%)	1.5E-13 (1.1%)	1.8E-11 (3.7%)	2.8E-07 (0.0%)
Molybdenum (Air/low. pop., long-term)	0.0E+00 (0.0%)	7.5E-12 (1.4%)	3.0E-07 (0.0%)	0.0E+00 (0.0%)	9.0E-12 (1.8%)	3.6E-07 (0.0%)
Nickel (Air/high. pop.)	9.8E-14 (0.7%)	5.5E-15 (0.0%)	8.7E-05 (0.0%)	9.5E-14 (0.7%)	5.3E-15 (0.0%)	8.4E-05 (0.0%)
Nickel (Air/low. pop., long-term)	1.6E-13 (1.2%)	9.3E-15 (0.0%)	1.7E-04 (0.0%)	2.1E-13 (1.5%)	1.2E-14 (0.0%)	2.1E-04 (0.0%)
Nickel (Air/low. pop.)	1.0E-12 (7.4%)	5.9E-14 (0.0%)	1.0E-03 (0.0%)	8.3E-13 (5.9%)	4.7E-14 (0.0%)	8.3E-04 (0.0%)
Silver (Air/low. pop., long-term)	0.0E+00 (0.0%)	3.3E-12 (0.6%)	7.4E-06 (0.0%)	0.0E+00 (0.0%)	4.1E-12 (0.8%)	9.2E-06 (0.0%)
Zinc (Air/low. pop., long-term)	0.0E+00 (0.0%)	1.2E-11 (2.3%)	1.3E-04 (0.0%)	0.0E+00 (0.0%)	1.5E-11 (3.1%)	1.6E-04 (0.0%)
Zinc (Air/low. pop.)	0.0E+00 (0.0%)	2.4E-11 (4.6%)	2.5E-04 (0.0%)	0.0E+00 (0.0%)	2.1E-11 (4.2%)	2.1E-04 (0.0%)
Zinc (Air/)	0.0E+00 (0.0%)	5.1E-12 (1.0%)	5.5E-05 (0.0%)	0.0E+00 (0.0%)	4.3E-12 (0.9%)	4.7E-05 (0.0%)
Copper (Water/ground water, long- term)	0.0E+00 (0.0%)	0.0E+00 (0.0%)	3.0E+01 (99.3%)	0.0E+00 (0.0%)	0.0E+00 (0.0%)	2.4E+01 (99.1%)
Cadmium (Soil/agricultural)	7.0E-14 (0.5%)	1.9E-11 (3.6%)	9.1E-05 (0.0%)	7.0E-14 (0.5%)	1.9E-11 (3.8%)	9.1E-05 (0.0%)

substance (compartment/ subcompartment)	low nuclear electricity mix			high nuclear electricity mix		
	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.d ay	human cancer (contribution%) / cases	human non-cancer (contribution%) / cases	eco (contribution%) / PAF.m3.d ay
Lead (Soil/agriculture)	9.6E-15 (0.1%)	3.4E-12 (0.6%)	2.6E-08 (0.0%)	9.6E-15 (0.1%)	3.4E-12 (0.7%)	2.5E-08 (0.0%)
Mercury (Soil/agriculture)	2.3E-14 (0.2%)	2.7E-12 (0.5%)	9.9E-09 (0.0%)	2.3E-14 (0.2%)	2.7E-12 (0.6%)	9.9E-09 (0.0%)
Zinc (Soil/agriculture)	0.0E+00 (0.0%)	3.0E-11 (5.8%)	1.1E-04 (0.0%)	0.0E+00 (0.0%)	3.0E-11 (6.2%)	1.1E-04 (0.0%)

SI VI.4 Contribution analysis of processes

Tables SI VI.4.1, 2, 3 and 4 present the contribution analysis for the scenarios of high and low nuclear energy mixes. Figures SI VI.4.1, 2, 3 and 4 shows the connection between the activities with major contribution and the foreground processes. The results for the contribution analysis come from SimaPro[®] v8.2. Climate change was calculated based in IPCC 2013 GWP 100 which is the same source for the dynamic method. Toxicity was calculated using USEtox[®] 1.04. For this reason, these results cannot be compared with the results obtained in the dynamic method as it was based in USEtox[®] 2. A cut-off of 1% was performed in order to keep only the processes which contributed the most.

Climate change

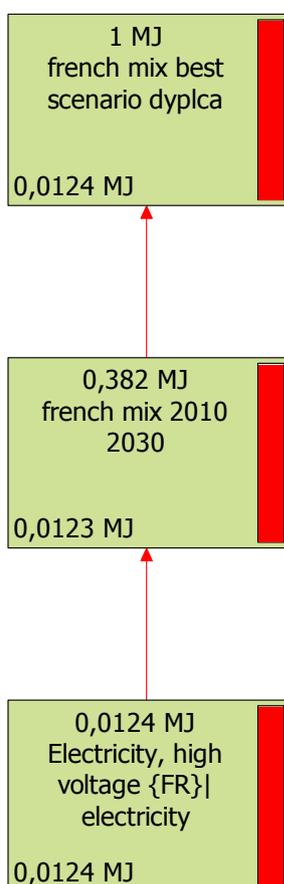


Figure VI.4.1 – Process contribution to the foreground processes; hard coal electricity source for the French electricity mix.

Electricity from hard coal is the process which contributes the most for climate change. This process is present in the mix for the period between 2010 and 2030 and the share is the same for both scenarios. For this reason, no important differences can be seen between both scenarios.

Table SI.VI.4.1 – Process contribution for conventional climate change (GWP100).

Process	Unit	French mix low nuclear scenario DyPLCA	French mix high nuclear scenario DyPLCA
Total of all processes	kg CO2 eq	1.4E-02	1.3E-02
Remaining processes	kg CO2 eq	5.8E-03	5.5E-03
Electricity, high voltage {FR} electricity production, hard coal Alloc Def, U	kg CO2 eq	3.1E-03	3.1E-03
Electricity, high voltage {FR} electricity production, oil Alloc Def, U	kg CO2 eq	9.7E-04	9.7E-04
Electricity, high voltage {FR} electricity production, natural gas, combined cycle power plant Alloc Def, U	kg CO2 eq	9.2E-04	9.2E-04
Hard coal {WEU} mine operation Alloc Def, U	kg CO2 eq	6.1E-04	6.1E-04
Electricity, for reuse in municipal waste incineration only {FR} treatment of municipal solid waste, incineration Alloc Def, U	kg CO2 eq	5.3E-04	5.3E-04
Hard coal {CN} mine operation Alloc Def, U	kg CO2 eq	4.0E-04	3.8E-04
Heat, central or small-scale, other than natural gas {RoW} heat production, anthracite, at stove 5-15kW Alloc Def, U	kg CO2 eq	2.5E-04	2.5E-04
Pig iron {GLO} production Alloc Def, U	kg CO2 eq	2.4E-04	2.1E-04
Heat, district or industrial, other than natural gas {RoW} heat production, at hard coal industrial furnace 1-10MW Alloc Def, U	kg CO2 eq	2.3E-04	2.3E-04
Clinker {RoW} production Alloc Def, U	kg CO2 eq	2.0E-04	1.7E-04
Diesel, burned in diesel-electric generating set, 10MW {GLO} diesel, burned in diesel-electric generating set, 10MW Alloc Def, U	kg CO2 eq	1.7E-04	2.0E-04
Uranium, enriched 3.8%, per separative work unit {US} uranium production, diffusion, enriched 3.8% Alloc Def, U	kg CO2 eq	1.3E-04	1.5E-04

Toxicity

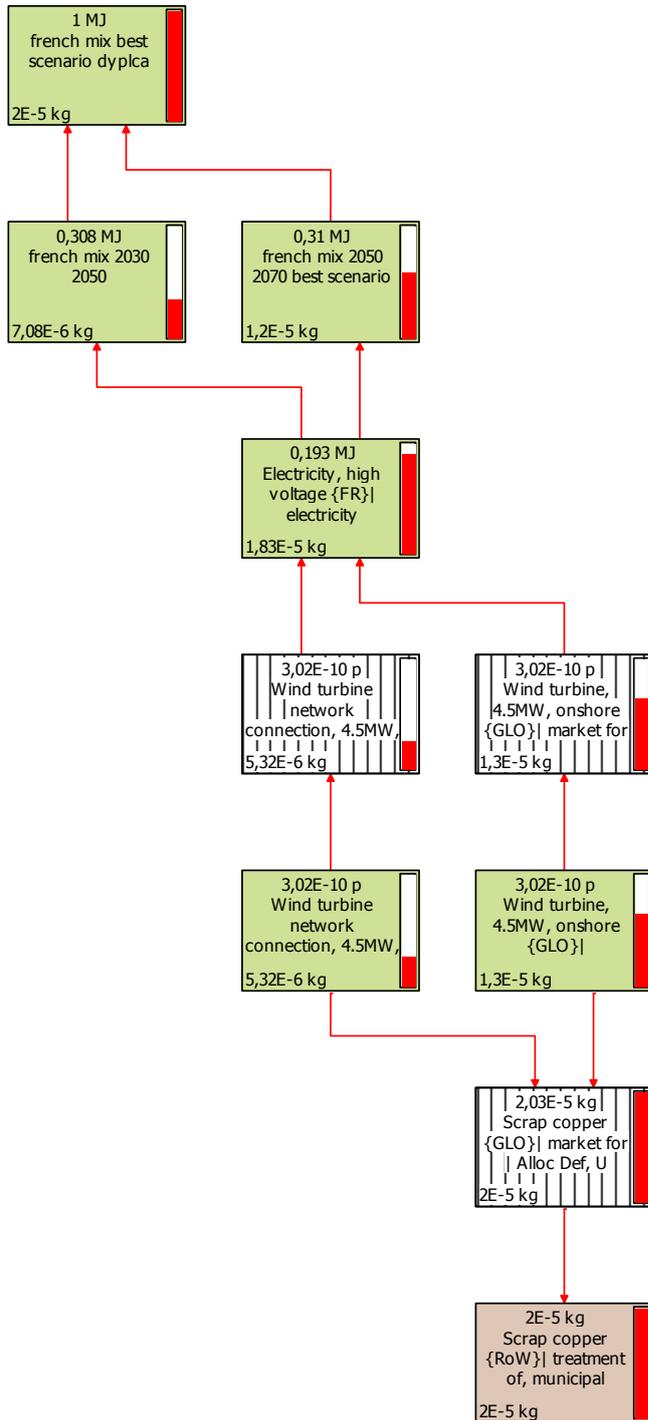


Figure SI VI.4.2 – Process contribution to the foreground processes; scrap copper treatment for the wind source of energy.

Table SI VI.4.2 – Process contribution for conventional ecotoxicity.

Process	Unit	French mix low nuclear scenario DyPLCA	French mix high nuclear scenario DyPLCA
Total of all processes	CTUe	8.7E-01	1.1E+00
Remaining processes	CTUe	6.0E-02	6.4E-02
Scrap copper {RoW} treatment of, municipal incineration Alloc Def, U	CTUe	6.0E-01	7.6E-01
Sulfidic tailing, off-site {GLO} treatment of Alloc Def, U	CTUe	8.2E-02	1.0E-01
Scrap steel {RoW} treatment of scrap steel, municipal incineration Alloc Def, U	CTUe	6.9E-02	8.4E-02
Uranium tailing, non-radioactive emission {GLO} treatment of Alloc Def, U	CTUe	3.4E-02	2.8E-02
Scrap steel {CH} treatment of, municipal incineration with fly ash extraction Alloc Def, U	CTUe	1.2E-02	1.4E-02
Scrap copper {CH} treatment of, municipal incineration with fly ash extraction Alloc Def, U	CTUe	9.1E-03	1.2E-02

Major contributor process in ecotoxicity impact is the treatment of scrap copper. The major source of this material is the wind power plants at the end of the lifetime of the infrastructure. This source of energy is found in all three periods analyzed in this study. The presence of this source of energy is more important in the scenario with low nuclear use which is reflected in the results of ecotoxicity.

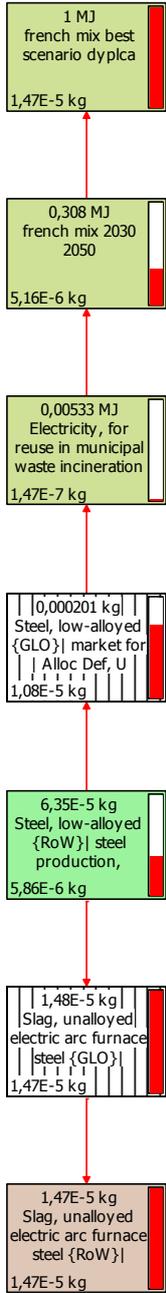


Figure SI VI.4.3 – Process contribution to the foreground processes; slag treatment in the municipal waste incineration source of energy.

Major contributor processes in human cancer toxicity impact is the treatment of slag. The major source of slag is the municipal waste incineration plants in the end of the lifetime of the infrastructure. This source of energy is found in all three periods analyzed in this study.

Table SI VI.4.3 – Process contribution for conventional human cancer toxicity.

Process	Unit	French mix low nuclear scenario DyPLCA	French mix high nuclear scenario DyPLCA
Total of all processes	CTUh	1.3E-09	1.4E-09
Remaining processes	CTUh	7.3E-11	7.8E-11
Slag, unalloyed electric arc furnace steel {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	3.5E-10	4.1E-10
Uranium tailing, non-radioactive emission {GLO} treatment of Alloc Def, U	CTUh	2.0E-10	1.7E-10
Sulfidic tailing, off-site {GLO} treatment of Alloc Def, U	CTUh	1.2E-10	1.5E-10
Basic oxygen furnace waste {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	1.0E-10	1.1E-10
Spoil from hard coal mining {GLO} treatment of, in surface landfill Alloc Def, U	CTUh	9.9E-11	1.0E-10
Spoil from lignite mining {GLO} treatment of, in surface landfill Alloc Def, U	CTUh	9.7E-11	9.7E-11
Sludge from steel rolling {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	5.5E-11	6.3E-11
Residue from Na-dichromate production {RoW} treatment of residue from Na-dichromate production, residual material landfill Alloc Def, U	CTUh	5.2E-11	5.2E-11
Redmud from bauxite digestion {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	4.9E-11	6.0E-11
Coal slurry {GLO} treatment of, impoundment Alloc Def, U	CTUh	4.8E-11	4.8E-11
Digester sludge {GLO} treatment of digester sludge, municipal incineration Alloc Def, U	CTUh	2.1E-11	2.1E-11
Dust, unalloyed electric arc furnace steel {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	1.9E-11	2.2E-11
Dust, alloyed electric arc furnace steel {RoW} treatment of, residual material landfill Alloc Def, U	CTUh	1.7E-11	1.6E-11

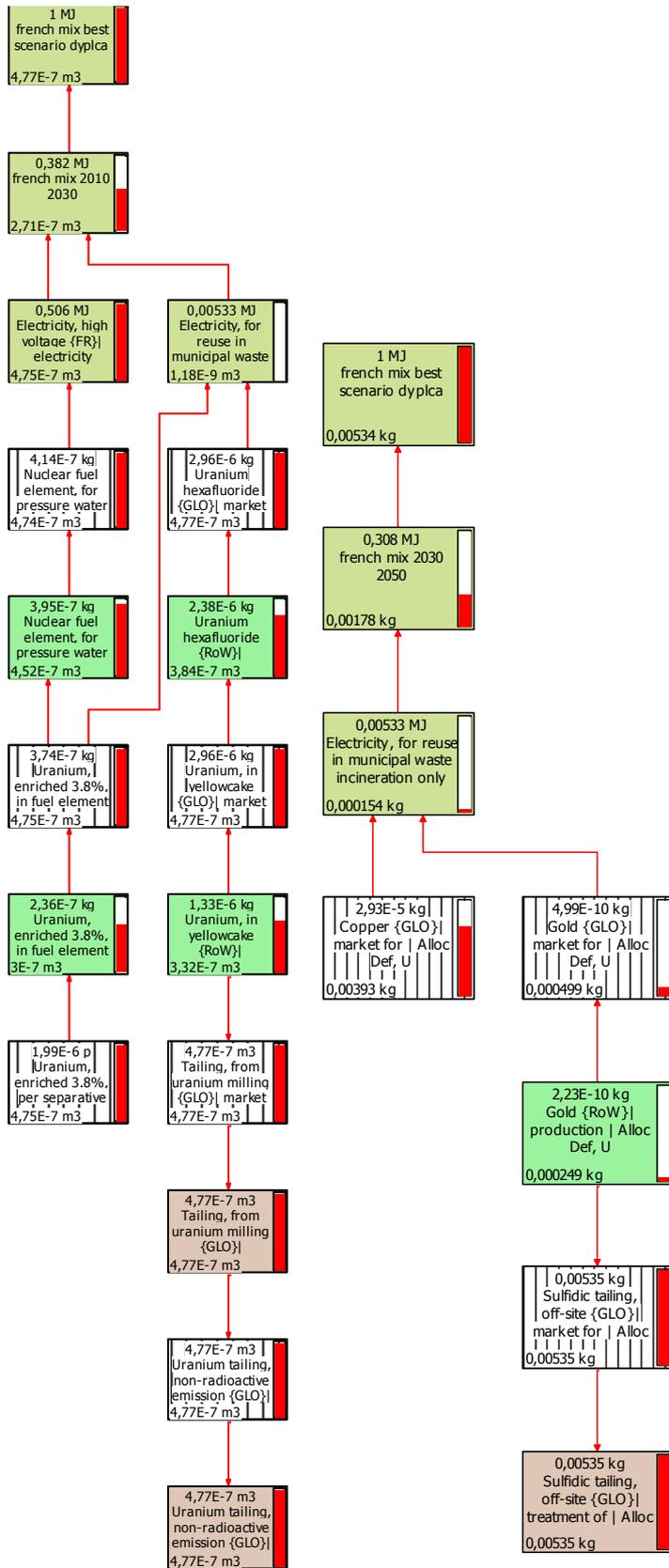


Figure SI VI.4.4 – Process contribution to the foreground processes; uranium tailing treatment for the nuclear source of energy and sulfidic tailing treatment for municipal source of energy.

Major contributor processes in human non-cancer toxicity impact are the treatment of uranium tailing and sulfidic tailing. The major source of uranium tailing is the nuclear power plants at the end of the lifetime of the infrastructure. This source of energy is found in all three periods analyzed in this study. The presence of this source of energy is more important in the scenario with high nuclear use. Also, the major source of sulfidic tailing is the incineration in municipal waste plants. This source of energy is also found in all three periods analyzed in this study.

Table SI VI.4.4 – Process contribution for conventional human non-cancer toxicity.

Process	Unit	French mix low nuclear scenario DyPLCA	French mix high nuclear scenario DyPLCA
Total of all processes	CTUh	1.1E-08	1.2E-08
Remaining processes	CTUh	1.2E-09	1.4E-09
Uranium tailing, non-radioactive emission {GLO} treatment of Alloc Def, U	CTUh	3.9E-09	3.2E-09
Sulfidic tailing, off-site {GLO} treatment of Alloc Def, U	CTUh	3.5E-09	4.3E-09
Wood ash mixture, pure {RoW} treatment of wood ash mixture, pure, landfarming Alloc Def, U	CTUh	4.2E-10	4.2E-10
Electricity, high voltage {FR} heat and power co-generation, biogas, gas engine Alloc Def, U	CTUh	4.0E-10	4.0E-10
Uranium, in yellowcake {GLO} uranium production, in yellowcake, in-situ leaching Alloc Def, U	CTUh	3.2E-10	2.7E-10
Spoil from hard coal mining {GLO} treatment of, in surface landfill Alloc Def, U	CTUh	2.8E-10	2.9E-10
Spoil from lignite mining {GLO} treatment of, in surface landfill Alloc Def, U	CTUh	2.8E-10	2.7E-10
Electricity, high voltage {FR} electricity production, hard coal Alloc Def, U	CTUh	2.1E-10	2.1E-10
Copper {RAS} production, primary Alloc Def, U	CTUh	1.6E-10	2.0E-10
Copper {RoW} production, primary Alloc Def, U	CTUh	1.5E-10	1.9E-10
Coal slurry {GLO} treatment of, impoundment Alloc Def, U	CTUh	1.5E-10	1.5E-10
Copper {RLA} production, primary Alloc Def, U	CTUh	1.4E-10	1.7E-10
Electricity, high voltage {FR} heat and power co-generation, wood chips, 6667 kW, state-of-the-art 2014 Alloc Def, U	CTUh	1.3E-10	1.3E-10
Steel, low-alloyed {RoW} steel production, electric, low-alloyed Alloc Def, U	CTUh	1.2E-10	1.4E-10

SI VII DyPLCA dynamic LCIA code documentation

This document contains some basic documentation for the dynamic life cycle impact assessment method for the DyPLCA project. It contains the dynamic methods for the calculation of climate change and toxicity. Moreover, it gives support modules to run the dynamic model and create files with results and graphics.

The code was developed in Python 2.7 and it is composed by 5 different modules: *main*, *substances_classes*, *climate_change*, *toxicity* and *generic_functions*.

The modules are explained hereafter:

The *main* module

The *main* module imports the results from DyPLCA inventory and adapts it for use in Python. Also the user inputs for the calculation of the dynamic impact assessment are given. Once the user has chosen the parameters, this module will create the folders to store all the results (csv files and graphics) and also it will call the modules *climate_change* and *toxicity* to perform the calculation. This is the module which is called by Python in order to run the all the model.

Information about the dynamic inventory can be found in (Tiruta-Barna et al., 2016) and in Chapter II. Also, the web app is found in <http://dypca.pigne.org/> or <http://dypca.univ-lehavre.fr/>.

The *substances_classes* module

This module presents the classes for the substances considered in the study. It contains three classes: *Dypca_substances* (it considers the substances which comes from the DyPLCA dynamic inventory), *Cc_substances* (it considers the substances which will be used for the calculation of climate change dynamic impact) and *Toxicity_substances* (it considers the substances which will be used for the calculation of the toxicity impact)

The *climate_change* module

This module contains the methods needed for the calculation of the dynamic climate change method.

The model is based in data found in IPCC (Intergovernmental Panel on Climate Change) website and reports. More information can be found in (IPCC, 2013) and in chapter III.

An application in a case study can be found in the (Shimako et al., 2016).

The *toxicity* module

This module contains the methods needed for the calculation of the dynamic toxicity model.

The model is based in the USEtox 2.0 toxicity model that can be found in <http://www.usetox.org/>. All data used for the toxicity calculation (matrices and substances) are available in this model. More information can be found in (Jolliet et al. 2006; Ligthart et al. 2004; McKone et al. 2006) and in chapter IV.

More information about the method can be found in the (Shimako et al., 2017)

The *generic_functions* module

This module contains the methods used for support of others modules. Functions for the creation of a csv document of graphics are presented here. As these functions do not have direct influence in the results of the models, they will not be described in this document.

Flowcharts for the classes and functions are presented in this document. Input and output data from the functions and classes are not exhaustively described in the flowcharts in order to simplify the description. More specific data can be found in the description of the functions and classes.

In order to run this project, the following components are needed:

- Microsoft Excel (for the extraction of substance information on-the-fly from the USEtox tool),
- the win32com package for Python, allowing the interaction with Excel,
- the matplotlib library which allows plotting
- the scipy library which is an ecosystem for mathematics, science, and engineering
- the numpy library which is used for scientific computing

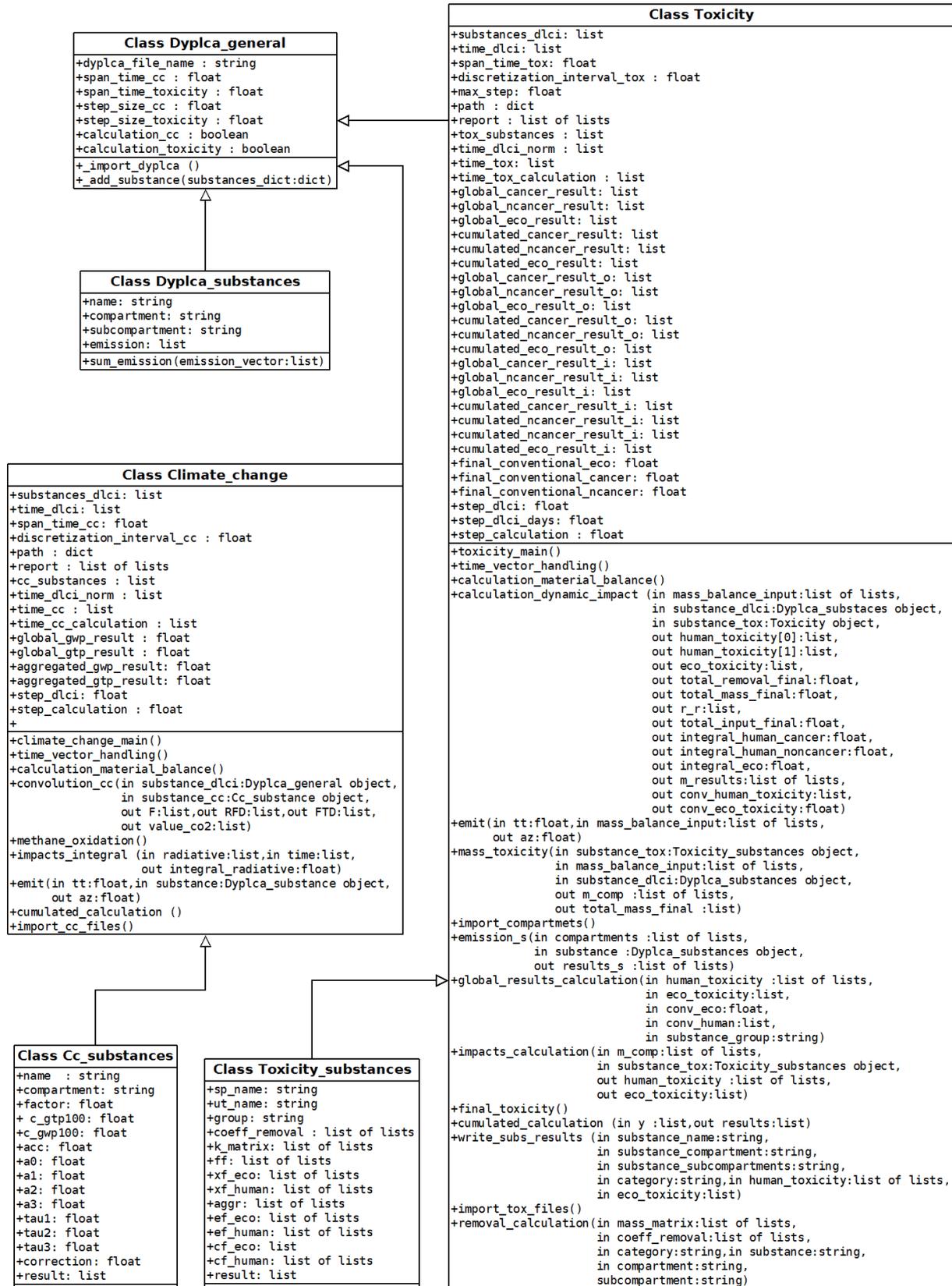


Figure SI.VII.1 – UML representation of the dynamic impact assessment model

SI VII.1 main module

It contains the method responsible for handling the data which comes from the DyPLCA dynamic inventory. Also, it reads the user parameters for the calculation of climate change and toxicity and calls these methods.

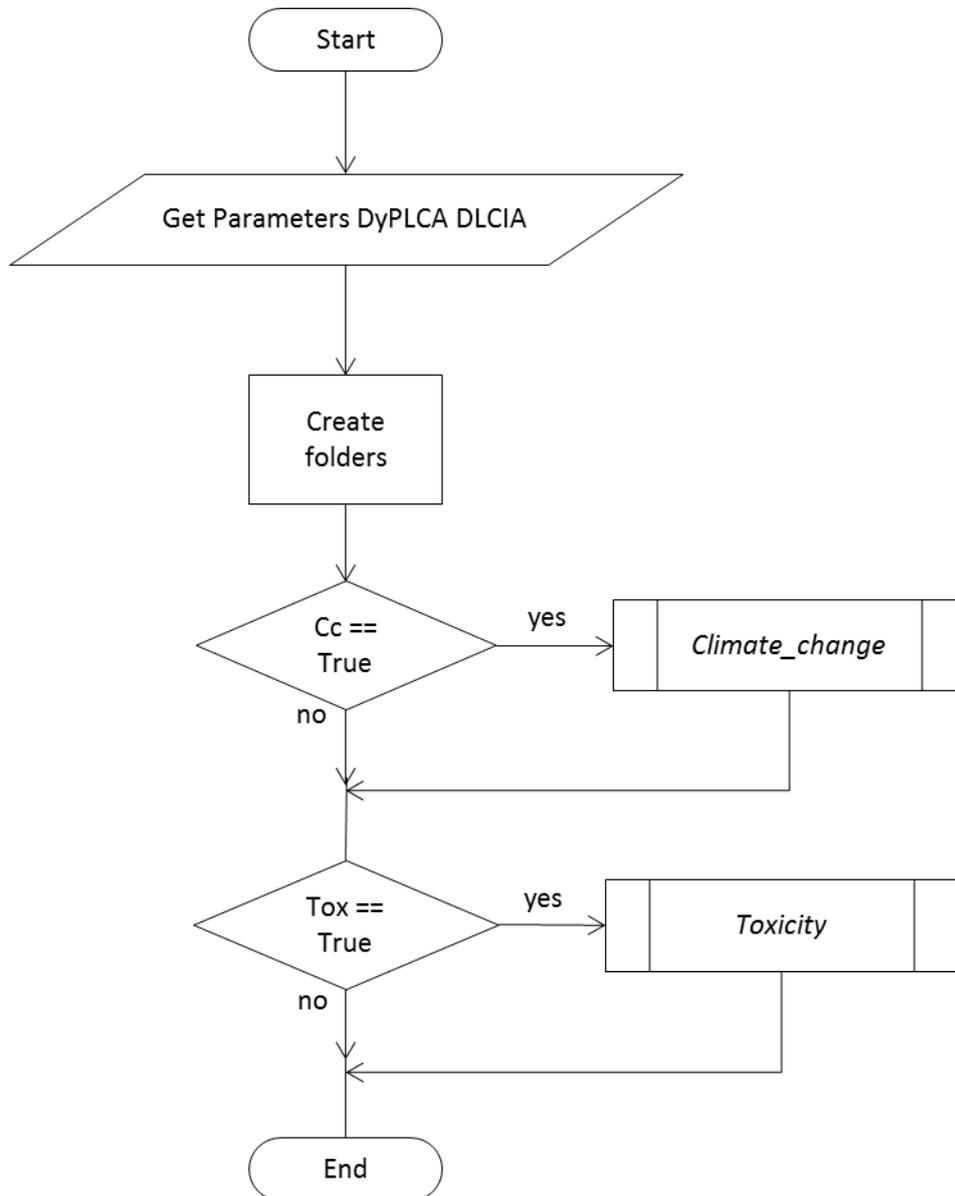


Figure SI.VII.2 – Flowchart representation of the main module

main(dypzca_params)

Runs the importation of DLCI results and also run the chosen DLCIA models.

The input parameter *dypzca_params* is a dictionary which contains the following elements:

Parameter	Type	Description
dypzca_file_name	string	Name of the DyPLCA file to be assessed
span_time_cc	float	Span time for climate change calculation
span_time_toxicity	float	Span time for toxicity calculation
step_size_cc	float	Time step size for cc (calculation and results display)
step_size_toxicity	float	Time step size for toxicity (results display)
calculation_cc	boolean	If true, it performs climate change calculation
calculation_toxicity	boolean	If true, it performs toxicity calculation

_create_project_folder (name):

It creates a folder *name* for the project. It can be found in the subfolder “results” in the python package folder.

Parameter	Type	Description
Name	string	Name for the folder, project name

_create_folder(category,_path):

It creates a folder *category* and others subfolders in the folder *_path*.

Parameter	Type	Description
category	string	Impact category name
path	string	Path in which the folder will be created

time_spent(start,stop,name):

This function calculates the time spent to run a DLCIA category *name* as the difference between the initial time *start* and the end time *stop*.

Parameter	Type	Description
name	string	Impact category name
start	float	Start time of calculation
stop	float	Stop time of calculation

class **Dyplca_general**(object):

Class used for DyPLCA dynamic inventory consideration.

The input parameters for this class comprise the following elements:

Parameter	Type	Description
dyplca_file_name	string	Name of the DyPLCA file to be assessed
span_time_cc	float	Span time for climate change calculation
span_time_toxicity	float	Span time for toxicity calculation
step_size_cc	float	Time step size for cc (calculation and results display)
step_size_toxicity	float	Time step size for toxicity (results display)
calculation_cc	boolean	If true, it performs climate change calculation
calculation_toxicity	boolean	If true, it performs toxicity calculation

_import_dyplca():

This function imports a DyPLCA dlc file. It imports the file with the name given by the parameter *dyplca_file_name*.

`_add_substance`(`substances_dict`):

Add substance dictionary *substances_dict* to the substance vector in the project class

Parameter	Type	Description
<code>substances_dict</code>	dict	It contains the data corresponding to a dlici substance

SI VII.2 substances_classes module

This module presents three classes for the following types of substances: inventory, climate change and toxicity.

Dyplca_general Class

class **Dyplca_general**(object):

Class used for DyPLCA dynamic inventory consideration.

The input parameters for this class comprise the following elements:

Parameter	Type	Description
name	string	Name of the substance in DLCI
compartment	string	Compartment of emission
subcompartment	string	Subcompartment of emission
emission	list	List with values of emission (kg/year)

sum_emission(*emission_vector*):

This function sums the input list *emission_vector* and the variable *emission* in a *Dyplca_general* object.

Parameter	Type	Description
<i>emission_vector</i>	list	List with values of emission (kg/year)

Cc_substances Class

class **Cc_substances**(object):

Class used for the climate change models' substances.

The input parameters for this class comprise the following elements:

Parameter	Type	Description
name	string	Name of the substance in climate change model
compartment	string	Compartment of emission
factor	float	Factor for impact calculation

c_gtp100	float	Conventional GTP100 value
c_gwp100	float	Conventional GWP100 value
acc	float	Specific radiative forcing
a0	float	IRF parameter a0
a1	float	IRF parameter a1
a2	float	IRF parameter a2
a3	float	IRF parameter a3
tau1	float	IRF parameter tau1
tau2	float	IRF parameter tau2
tau3	float	IRF parameter tau3
correction	float	Value for correction of impact
result	list	Results climate change

Toxicity_substances Class

class **Toxicity_substances(object):**

Class used for the toxicity models' substances.

The input parameters for this class comprise the following elements:

Parameter	Type	Description
sp_name	string	Name of the substance in SimaPro
ut_name	string	Name of the substance in USEtox
group	string	Substance group (organic or inorganic)
coeff_removal	list of lists	Matrix of coefficient for removal
k_matrix	list of lists	Matrix of k constants
ff	list of lists	Fate factor matrix
xf_eco	list of lists	Ecotoxicity exposure factor matrix
xf_human	list of lists	Human toxicity exposure factor matrix
aggr	list of lists	Aggregation matrix

ef_eco	list	Ecotoxicity effect factor matrix
ef_human	list of lists	Human toxicity effect factor matrix
cf_human	list of lists	Human toxicity characterization factor matrix
cf_eco	list of lists	Ecotoxicity characterization factor matrix
result	list	Results toxicity

SI VII.3 climate_change module

This module contains the methods needed for the calculation of the dynamic climate change method.

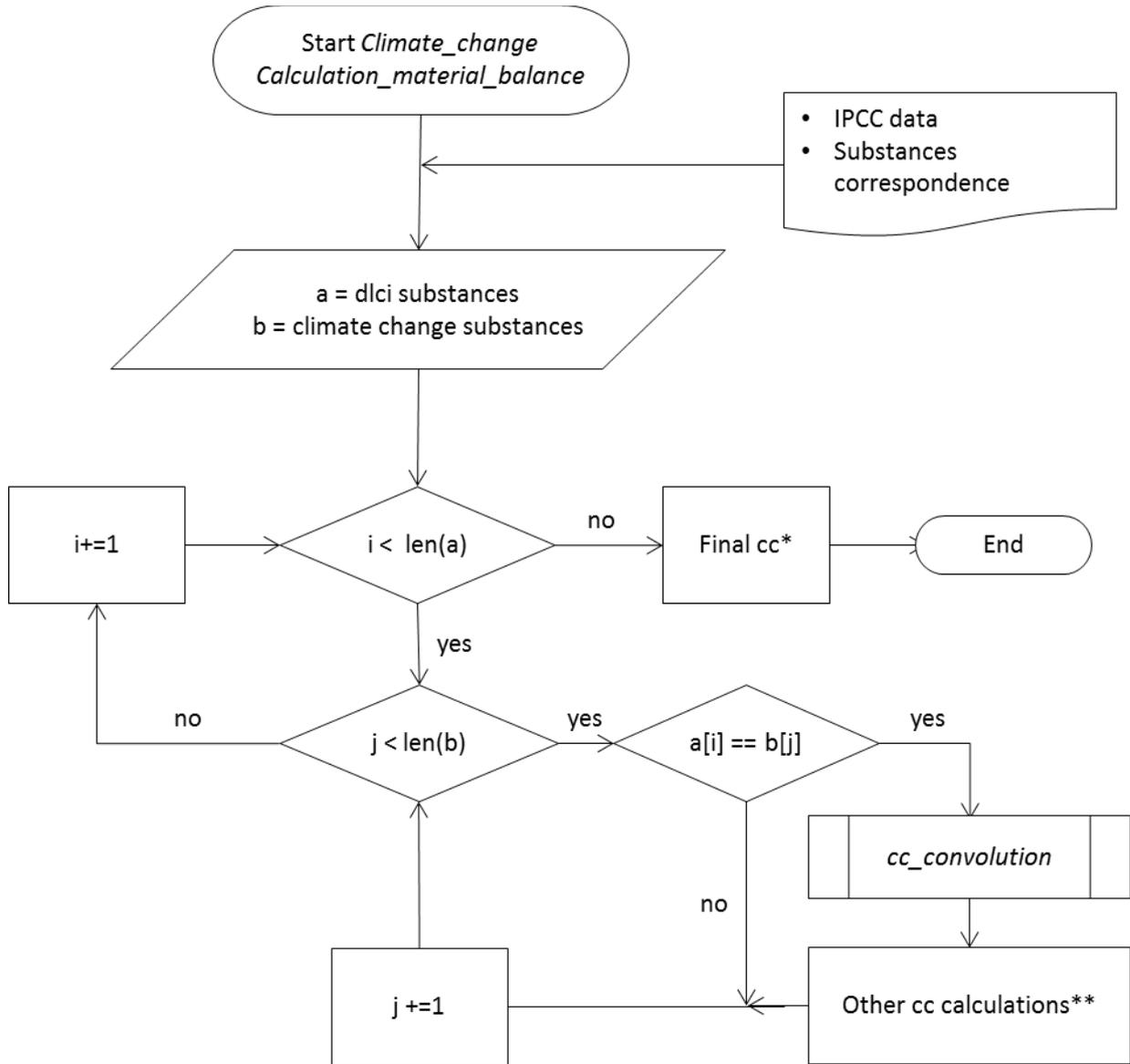


Figure SI.VII.3 –climate_change module flowchart representation.

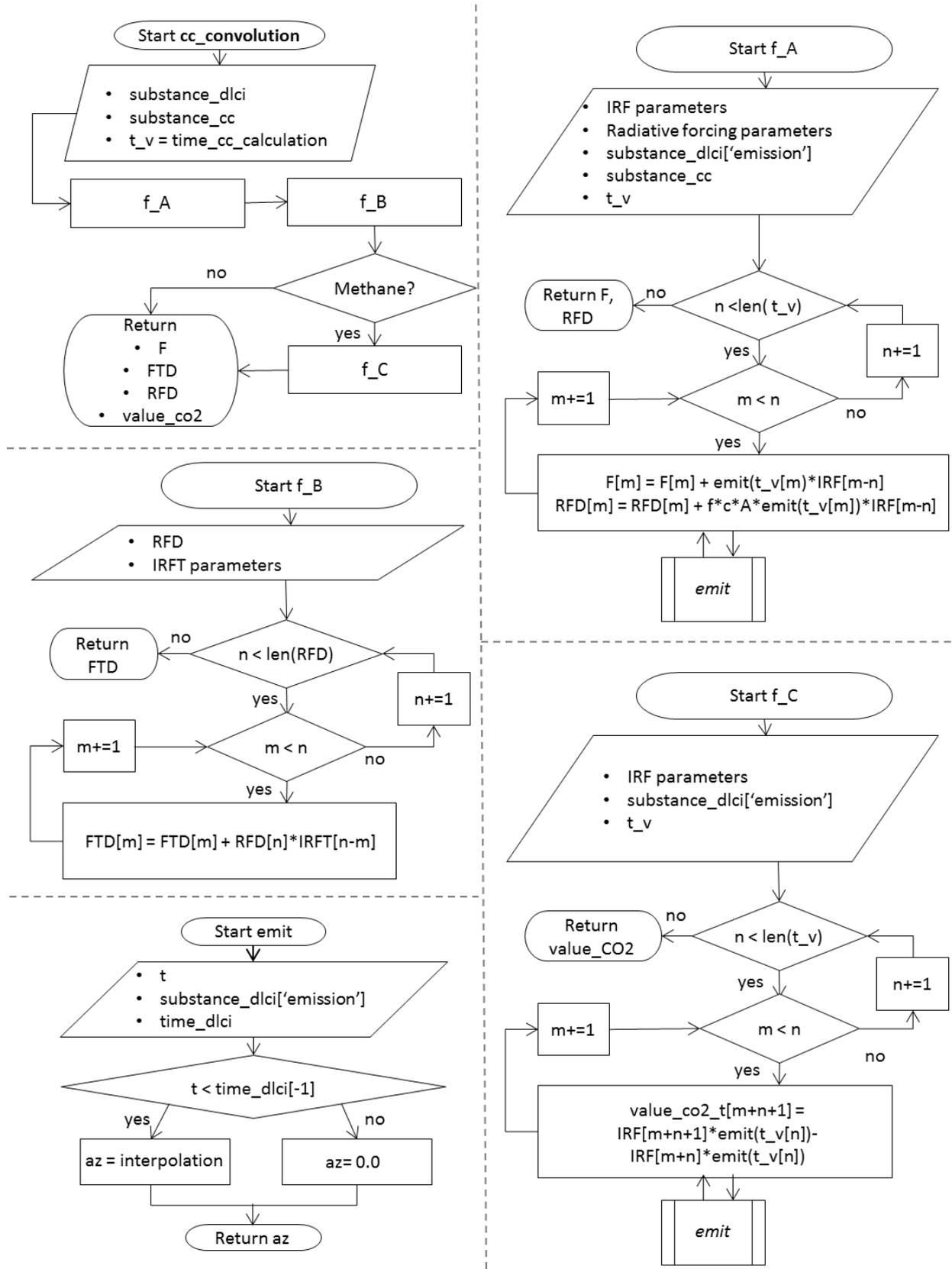


Figure SI.VII.4- cc_convolution method flowchart representation.

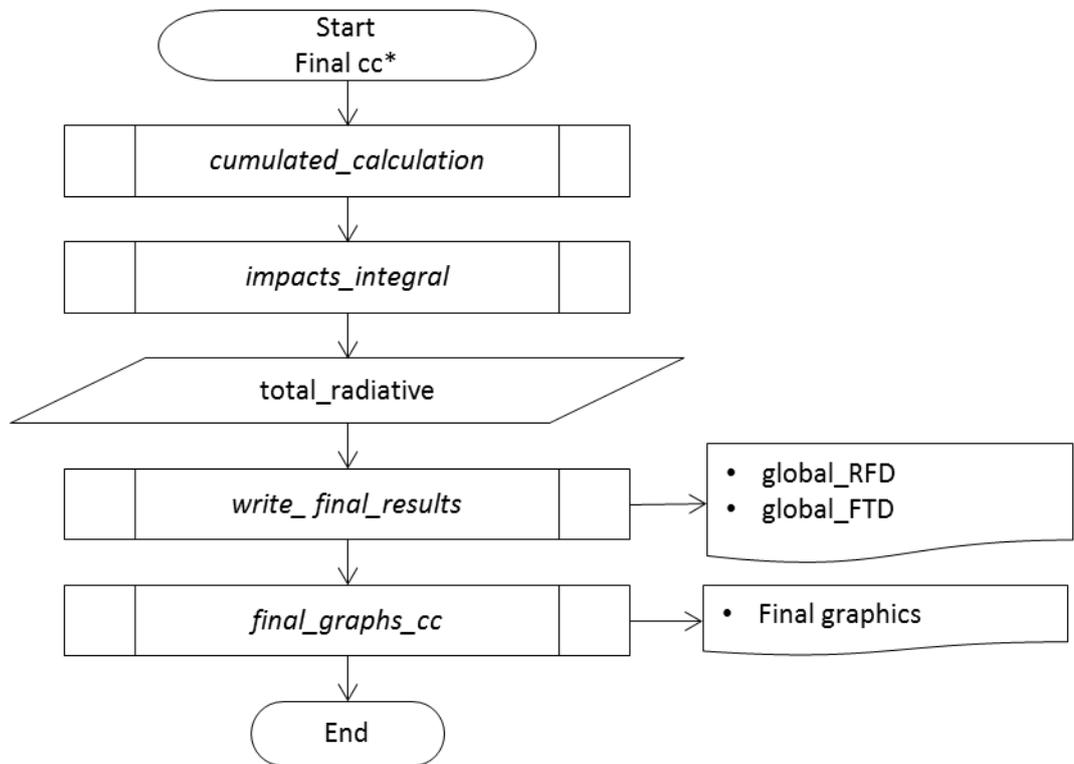
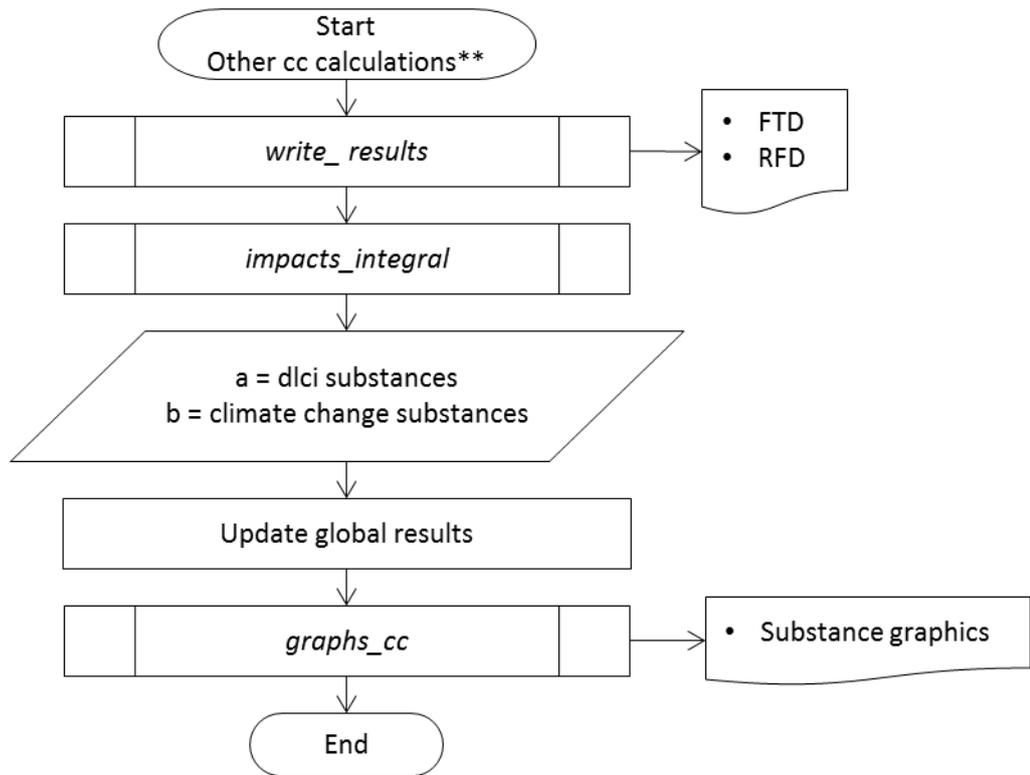


Figure SI.VII.5 – Support flowchart for figure SI.VII.3

class **Climate_change**(object):

Class used for dynamic climate change impact assessment calculation.

The input parameters for this class comprise the following elements:

Parameter	Type	Description
substances_dlci	list	List with substances of dlci
time_dlci	list	Time vector of dlci in years
span_time_cc	float	Span time for climate change calculation
discretization_interval_cc	float	Step for convolution
path	dict	Paths for saving results
report	list of lists	Give final report for climate change
cc_substances	list	List of substances for climate change method
time_dlci_norm	list	Time vector of dlci normalized
time_cc	list	Time vector for cc calculation (without normalization)
time_cc_calculation	list	Time vector for cc calculation (normalized)
global_gwp_result	float	Final dynamic result for radiative forcing
global_gtp_result	float	Final dynamic result for temperature
aggregated_gwp_result	float	Aggregated results for dynamic radiative forcing
aggregated_gtp_result	float	Aggregated results for dynamic temperature
step_dlci	float	Time step size of dlci
step_calculation	float	Time step size of climate change calculation

climate_change_main():

This function calls the main methods for the calculation of dynamic climate change.

time_vector_handling():

This function converts the imported parameters in day basis; it also normalizes the time vector to perform the calculations (avoid negative values in the time vector).

calculation_material_balance():

This function calculates the material balance and impacts. It searches the correspondence between substances in the DyPLCA inventory file and the substances in the dynamic climate change assessment and performs the calculations. It also includes a function for the calculation of the methane oxidation.

convolution_cc(substance_dlci,substance_cc):

This function calculates the convolution for the calculation of the *substance_dlci* burden, its dynamic radiative forcing and its dynamic temperature.

The input parameters for this method comprise the following elements:

Parameter	Type	Description
substance_dlci	list	List with substances of dlci
substance_cc	list	Time vector of dlci in years

This function returns:

Parameter	Type	Description
F	list	Results for the substance burden
FTD	list	Results for the dynamic temperature
RFD	list	Results for the dynamic radiative forcing
value_co2	list	Amount of CO ₂ to be add to inventory due to methane oxidation

methane_oxidation():

This function performs the convolution calculation and the impacts calculation when the substance is methane. It also adds the value of methane converted in CO₂ in the inventory for its further consideration in the assessment.

impacts_integral (radiative, time):

This function calculates the integral of the impact *radiative*.

Parameter	Type	Description
radiative	list	Vector with impact results

time	list	Time vector
------	------	-------------

This function returns:

Parameter	Type	Description
integral_radiative	float	Integral of the dynamic radiative forcing

emit(tt, substance):

This function calculates the dlcI inventory value that corresponds to a specific time by interpolation.

Parameter	Type	Description
tt	float	Point in time for interpolation
substance	Dyplca_substance object	dlcI substance (uses emission variable)

This function returns:

Parameter	Type	Description
az	float	Dynamic inventory value after interpolation

cumulated_calculation ():

This function calculated the cumulated vector for the global results of the climate change study. It considers the global vector for radiative forcing and calculates the final cumulated vector.

SI VII.4 toxicity module

This module contains the methods needed for the calculation of the dynamic toxicity model.

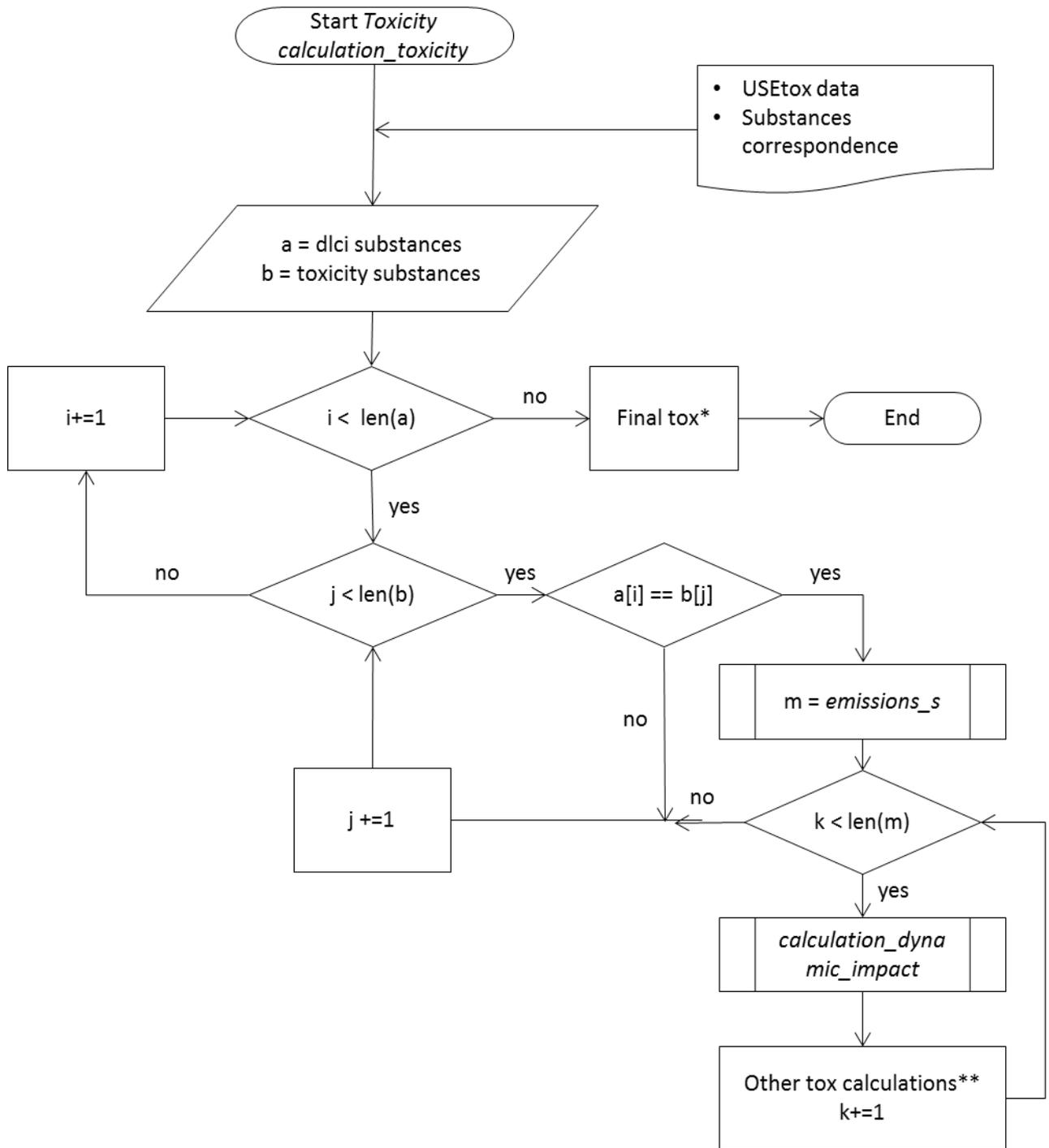


Figure SI.VII.6 –toxicity module flowchart representation.

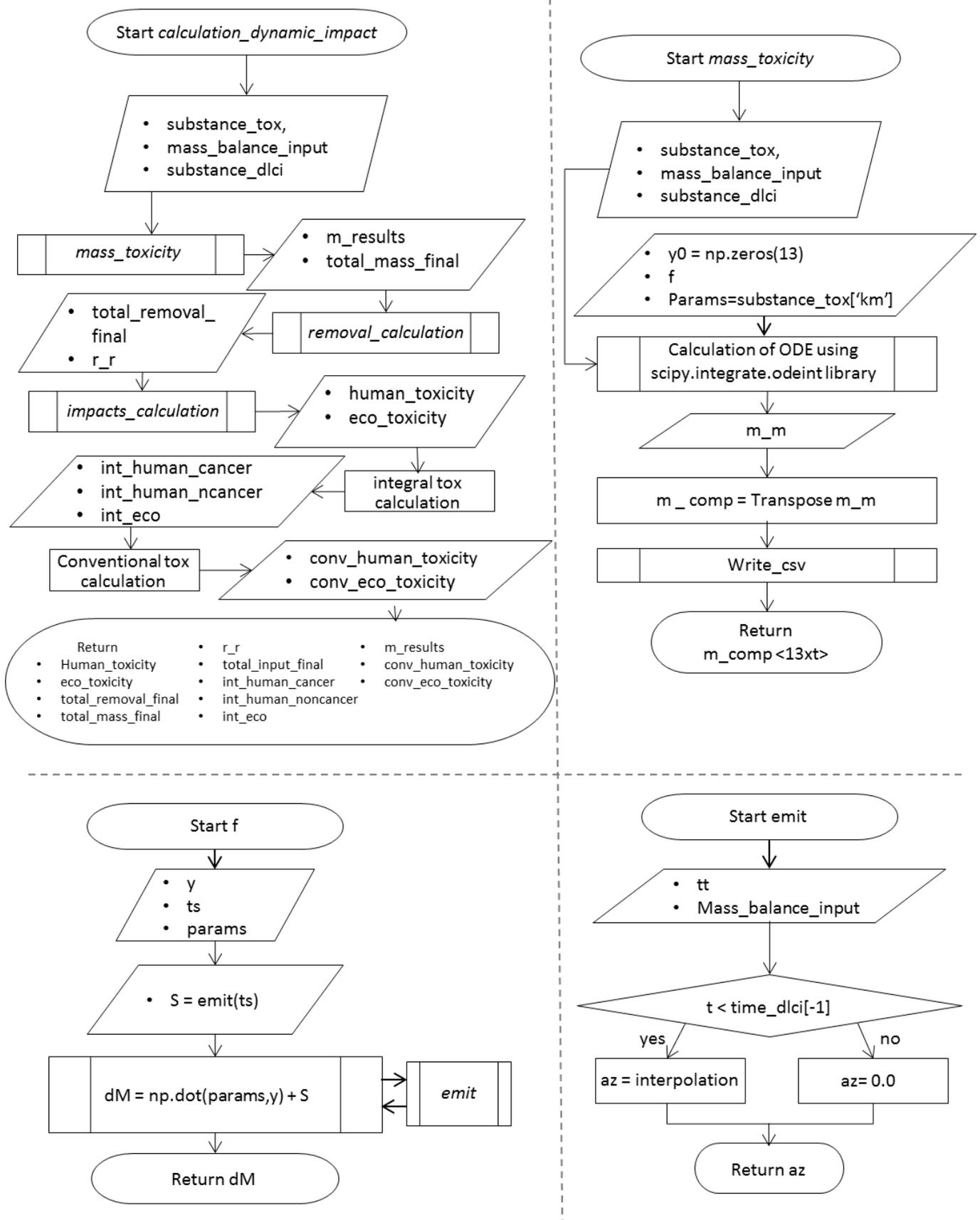


Figure SI.VII.7 –calculation_dynamic_impact method flowchart representation.

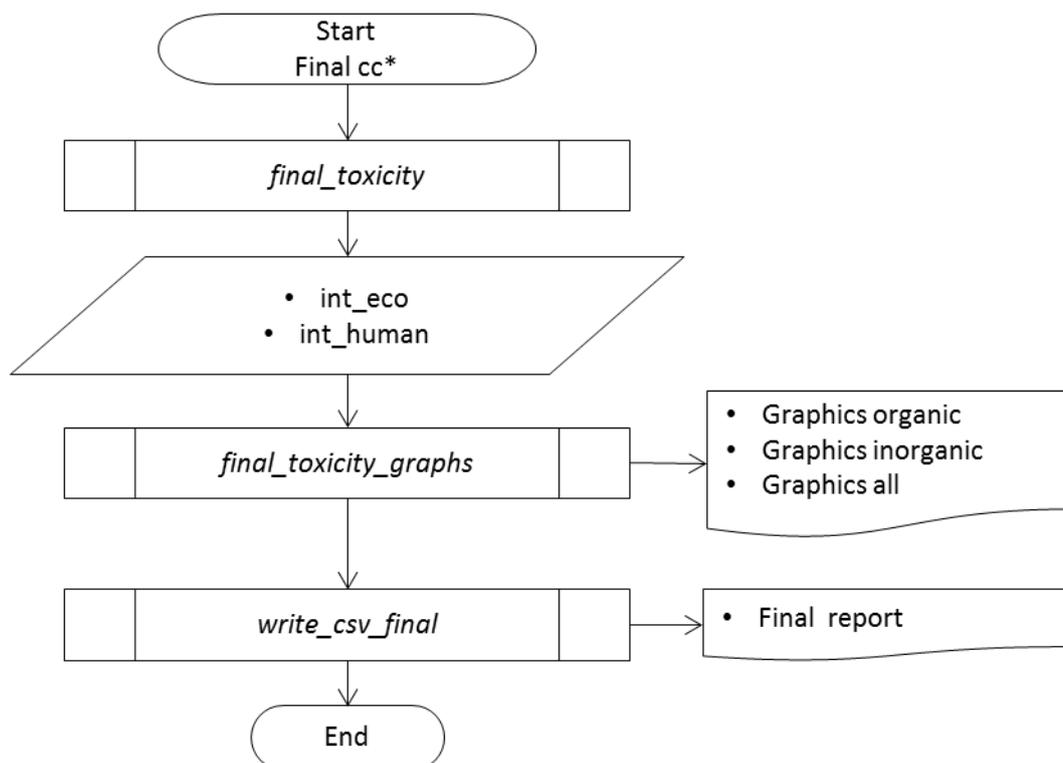
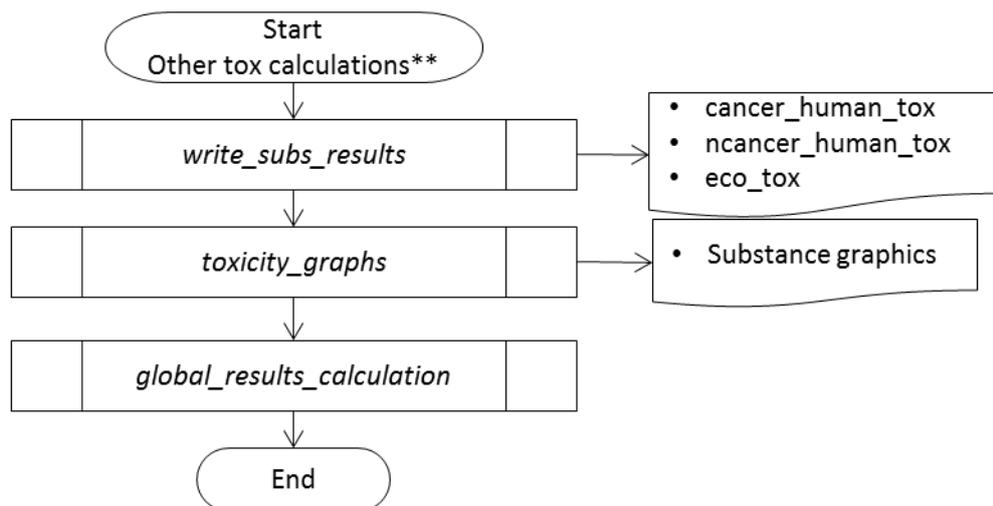


Figure SI.VII.8 – Support flowchart for figure SI.VII.6

class **Toxicity**(object):

Class used for dynamic toxicity impact assessment calculation.

The input parameters for this class comprise the following elements which are given in form of a dictionary:

Parameter	Type	Description
substances_dlci	list	List with substances of dlci
time_dlci	list	Time vector of dlci in years
span_time_tox	float	Span time for toxicity calculation
discretization_interval_tox	float	Step for results display
value_discretization	string	Method of mass balance resolution
max_step	float	Maximum step in case of solver in mass bal. resolution
path	dict	Paths for saving results
report	list of lists	Give final report for toxicity
tox_substances	list	List of substances for toxicity method
time_dlci_norm	list	Normalized vector of dlci time
time_tox	list	Time vector for toxicity calculation (w/out normalization)
time_tox_calculation	list	Time vector for toxicity calculation (normalized)
global_cancer_result	list	Final results for human cancer toxicity
global_ncancer_result	list	Final results for human non-cancer toxicity
global_eco_result	list	Final results for eco toxicity
cumulated_cancer_result	list	Cumulated results for human cancer toxicity
cumulated_ncancer_result	list	Cumulated results for human non-cancer toxicity
cumulated_eco_result	list	Cumulated results for eco toxicity
global_cancer_result_o	list	Final results for human cancer toxicity for organic substances.
global_ncancer_result_o	list	Final results for human non-cancer toxicity for organic substances.

global_eco_result_o	list	Final results for eco toxicity for organic substances.
cumulated_cancer_result_o	list	Cumulated results for human cancer toxicity for organic substances.
cumulated_ncancer_result_o	list	Cumulated results for human non-cancer toxicity for organic substances.
cumulated_eco_result_o	list	Cumulated results for eco toxicity for organic substances.
global_cancer_result_i	list	Final results for human cancer toxicity for inorganic substances.
global_ncancer_result_i	list	Final results for human non-cancer toxicity for inorganic substances.
global_eco_result_i	list	Final results for eco toxicity for inorganic substances.
cumulated_cancer_result_i	list	Cumulated results for human cancer toxicity for inorganic substances.
cumulated_ncancer_result_i	list	Cumulated results for human non-cancer.
cumulated_ncancer_result_i	list	Cumulated results for human non-cancer toxicity for inorganic substances.
cumulated_eco_result_i	list	Cumulated results for eco toxicity for inorganic substances.
final_conventional_eco	float	Final conventional results for eco toxicity.
final_conventional_cancer	float	Final conventional results for human cancer toxicity.
final_conventional_ncancer	float	Final conventional results for human non-cancer toxicity.
step_dlci	float	Time step size of dynamic LCI.
step_dlci_days	float	Time step size of dynamic LCI in days.
step_calculation	float	Time step size of dynamic toxicity calculation.

toxicity_main():

This function calls the main methods for the calculation of dynamic toxicity.

time_vector_handling():

This function converts the imported parameters in day basis; it also normalizes the time vector to perform the calculations (avoid negative values in the time vector).

calculation_toxicity():

This function calculates the dynamic toxicity (it uses USEtox® model data). It searches the correspondences between substances in the DyPLCA inventory file and the substance in the dynamic toxicity assessment and perform the calculations. It also breaks down the results in organic and inorganic substances.

calculation_dynamic_impact (mass_balance_input,substance_dhci,substance_tox):

This function returns a tuple of all dynamic impact values for a given substance (*substance_dhci,substance_tox*) and emission (*mass_balance_input*).

The input parameters for this function comprise the following elements:

Parameter	Type	Description
mass_balance_input	list of lists	Matrix with the emission (13 compartments)
substance_dhci	Dyplca_substaces object	Substance from dynamic LCI
substance_tox	Toxicity object	Substance with toxicity parameters

This function returns:

Parameter	Type	Description
human_toxicity[0]	list	Results for cancer human toxicity
human_toxicity[1]	list	Results for non-cancer human toxicity
eco_toxicity	list	Results for freshwater ecotoxicity
total_removal_final	float	Final value of substance mass removal
total_mass_final	float	Final value of substance remaining mass
r_r	list	Results for the removal of substance
total_input_final	float	Final value for input of substance
integral_human_cancer	float	Integral of human cancer toxicity results
integral_human_noncancer	float	Integral of human non-cancer toxicity results
integral_eco	float	Integral of ecotoxicity results
m_results	list of lists	Results of fate of a substance

conv_human_toxicity	list	Conventional human toxicity results (cancer and non-cancer)
conv_eco_toxicity	float	Conventional ecotoxicity results

emit(tt,mass_balance_input):

This function calculates the emission value (for a given emission *mass_balance_input*) that corresponds to a specific time *tt* by interpolation.

The input parameters for this function comprise the following elements:

Parameter	Type	Description
tt	float	Point in time for interpolation
mass_balance_input	list of lists	Emissions for interpolation

This function returns:

Parameter	Type	Description
az	float	Dynamic inventory value (found by interpolation)

mass_toxicity(substance_tox, mass_balance_input,substance_dlci):

This function calculates the mass balance which results on the dynamic fate for a substance (*substance_dlci*, *substance_tox*) and emission (*mass_balance_input*)

The input parameters for this function comprise the following elements:

Parameter	Type	Description
substance_tox	Toxicity_substances object	Substance of toxicity method
mass_balance_input	list of lists	Emissions for the calculation of the fate
substance_dlci	Dyplca_substances object	Substances of the DyPLCA inventory

This function returns:

Parameter	Type	Description
m_comp	list of lists	Fate of the substance in compartments
total_mass_final	list	Final remaining mass of substance in compartments

import_compartments():

This function imports the compartments for the toxicity model

emission_s(substance, compartments):

This function returns a vector of vector which adapted for the use in the material balance calculation. The emission of *substance* in certain environmental media (present in *compartments*) from DLCI is inputted in one vector which corresponds to the compartment of emission and the other vectors for other compartments have zeros.

The input parameters for this function comprise the following elements:

Parameter	Type	Description
compartments	list of lists	Contains the data of compartments
substance	Dyplca_substances object	DyPLCA inventory substance

This function returns:

Parameter	Type	Description
results_s	list of lists	Allocate the emission form dlci to one specific compartment, others compartments contains zeros.

global_results_calculation(human_toxicity, eco_toxicity, conv_eco, conv_human, substance_group):

This function updates the values of the global toxicity results. It sums the results of a specific substance (*human_toxicity*, *eco_toxicity*, *conv_eco*, *conv_human*) to the global value according to substance category (*substance_group*; organic or inorganic).

The input parameters for this function comprise the following elements:

Parameter	Type	Description
human_toxicity	list of lists	Vector of results for cancer and non-cancer human toxicity.
eco_toxicity	list	Vector of results for ecotoxicity.
conv_eco	float	Results of conventional ecotoxicity.
conv_human	list	Results of conventional human toxicity.
substance_group	string	Substance category: organic or inorganic.

impacts_calculation(*m_comp*,*substance_tox*):

This function calculates the dynamic impact of a certain fate *m_comp* for a substance *substance_tox*.

The input parameters for this function comprise the following elements:

Parameter	Type	Description
m_comp	list of lists	Matrix of resulting fate of substance
substance_tox	Toxicity_substances object	Provide the parameters for the impacts calculation

This function returns:

Parameter	Type	Description
human_toxicity	list of lists	Dynamic results for human toxicity
eco_toxicity	list	Dynamic results for ecotoxicity

final_toxicity ():

This function calculates the integral of human and ecotoxicity final results

cumulated_calculation (y):

This function calculates the cumulated profile of the impact described by y.

The input parameters for this function comprise the following elements:

Parameter	Type	Description
y	list	Impact (human cancer or non-cancer or ecotoxicity)

This function returns:

Parameter	Type	Description
results	list	Cumulated impact (human cancer or non-cancer or ecotoxicity)

write_subs_results (substance_name, substance_compartment, substance_subcompartment, category, human_toxicity, eco_toxicity):

This function writes the *human_toxicity* and *ecotoxicity* for a specific substance in an environmental media (*substance_name*, *category*, *substance_compartment*, *substance_subcompartment*) in csv files.

Parameter	Type	Description
substance_name	string	Name of the substance
substance_compartment	string	Compartment of emission
substance_subcompartments	string	Subcompartment of emission
category	string	Organic or inorganic
human_toxicity	list of lists	Vector of human toxicity results
eco_toxicity	list	Vector of ecotoxicity results

import_tox_files():

This function imports the matrices from USEtox. It uses the os library to access the values calculated by USEtox 2.0 tool reference. It can also import from a pkl file through the pickle library data was previously saved.

removal_calculation(mass_matrix, coeff_removal, substance, compartment, subcompartment):

This function calculates the removal of certain substance emitted in an environmental media (*substance, compartment, subcompartment*) returns the total mass removed from the system. Also create graphics for the removal per compartment and total removal.

Parameter	Type	Description
mass_matrix	list of lists	Fate results for a substance
coeff_removal	list of lists	Matrix of removal coefficients
category	string	Category of substance (organic or inorganic)
substance	string	Name of substance
compartment	string	Compartment of emission
subcompartment	string	Subcompartment of emission

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English abstract

Life Cycle Assessment (LCA) is a widely used method for the environmental evaluation of an anthropogenic system. However, LCA scholars pointed out the lack of a temporal dimension as a limitation. The processes of technosphere are dynamic which leads to a time dependent life cycle inventory (LCI). Environmental mechanisms involved in impact developments have distinct dynamic behaviors determining specific temporal occurrence. However, the current life cycle impact assessment (LCIA) methods consider arbitrarily fixed time horizons and/or steady state conditions. The objective of this thesis is to contribute to the development of an operational methodology and adapted tools for the consideration of time dependency in LCA, with emphasis on the development of an integrated modelling solution for both the life cycle inventory and the life cycle impact assessment phases. The first contribution of this thesis concerns the development of a temporal data base, leaning against ecoinvent data base, in which temporal parameters have been attributed to the data sets. Dynamic climate change and toxicity impacts were developed by adapting available models and were implemented in a homemade computational tool. The modelling approach takes into account the noisy nature of substance emissions in function of time as calculated by DyPLCA temporal LCI model.

Keywords: dynamic LCA, life cycle inventory, climate change, toxicity, ecotoxicity

Résumé en Français

L'analyse du cycle de vie (ACV) est une méthode très utilisée pour l'évaluation environnementale d'un système anthropique. Les spécialistes ont souligné l'absence de dimension temporelle comme une limitation. Les procédés de la technosphère sont dynamiques, ce qui conduirait à un inventaire de cycle de vie (ICV) dépendant du temps. Les mécanismes environnementaux impliqués dans la génération des impacts ont des caractéristiques dynamiques variées déterminant une manifestation temporelle spécifiques des impacts. Cependant, l'impact du cycle de vie (EICV) actuelles considère des modèles en conditions stationnaires et des horizons de temps arbitrairement fixés. L'objectif de cette thèse est de contribuer au développement d'une méthodologie opérationnelle et des outils adaptés pour la prise en compte du temps dans l'ACV, en accordant une importance au développement d'une approche de modélisation intégrée pour l'ICV et l'EICV. La première contribution de cette thèse concerne le développement d'une base de données temporelle, en s'appuyant sur la base de données ecoinvent, dans laquelle les paramètres temporels ont été attribués aux sets de données. Des indicateurs dynamiques pour le changement climatique et la toxicité ont été développés en adaptant les modèles disponibles et ils ont été mis en place dans un outil de calcul propre. L'approche de modélisation tient compte de la nature fluctuante des émissions des substances en fonction du temps calculées par le modèle d'ICV temporel DyPLCA.

Mots-clés: ACV dynamique, inventaire du cycle de vie, changement climatique, toxicité, ecotoxicité